

On boundary value problems for Dirac type operators. I. Regularity and self-adjointness

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ABSTRACT. In a series of papers, we will develop systematically the basic spectral theory of (self-adjoint) boundary value problems for operators of Dirac type. We begin in this paper with the characterization of (self-adjoint) boundary conditions with optimal regularity, for which we will derive the heat asymptotics and index theorems in subsequent publications. Along with a number of new results, we extend and simplify the proofs of many known theorems.

Our point of departure is the simple structure which is displayed by Dirac type operators near the boundary. Thus our proofs are given in an abstract functional analytic setting, generalizing considerably the framework of compact manifolds with boundary.

The results of this paper have been announced in [11].

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1. Introduction

1.A. The compact case. Let \widetilde{M} be a compact oriented Riemannian manifold of dimension m , $\widetilde{E} \rightarrow \widetilde{M}$ a hermitian vector bundle, and \widetilde{D} a symmetric elliptic differential operator of order $d \in \mathbb{Z}_+$ on $C^\infty(\widetilde{E})$. The classical results on existence, uniqueness, and regularity of solutions of \widetilde{D} are among the cornerstones of Global Analysis:

- \widetilde{D} is essentially self-adjoint in $L^2(\widetilde{E})$ with domain $C^\infty(\widetilde{E})$ (by slight abuse of notation, we denote the closure of \widetilde{D} by the same symbol); (1.1)

- \widetilde{D} is a Fredholm operator (of index 0), i.e. there are a bounded operator \widetilde{Q} and compact operators $\widetilde{K}_r, \widetilde{K}_l$ in $L^2(\widetilde{E})$ such that (1.2)

$$\widetilde{D}\widetilde{Q} = I - \widetilde{K}_r, \quad \widetilde{Q}\widetilde{D} = I - \widetilde{K}_l;$$

- with respect to the Sobolev scale $H_s(\widetilde{E}) := \mathcal{D}((\widetilde{D}^2 + I)^{s/2d})$, $s \geq 0$, (1.3)
- \widetilde{Q} is of order $-d$ and $\widetilde{K}_{r/l}$ of order $-\infty$.

The restriction to symmetric operators is not essential since we may always consider a given elliptic operator together with its adjoint. But it is a technical advantage for more refined questions like index theorems: We bring in an isometric involution, $\widetilde{\omega}$, on \widetilde{E} which anticommutes with \widetilde{D} on $C^\infty(\widetilde{E})$ and hence produces a splitting

$$\widetilde{D} = \begin{pmatrix} 0 & \widetilde{D}_- \\ \widetilde{D}_+ & 0 \end{pmatrix} \text{ on } C^\infty(\widetilde{E}_+) \oplus C^\infty(\widetilde{E}_-), \quad (1.4)$$

with \widetilde{E}_\pm the ± 1 -eigenbundle of $\widetilde{\omega}$. Then, by the well-known formula of McKean-Singer we have

$$\text{ind } \widetilde{D}_+ = \text{tr}[\widetilde{\omega} e^{-t\widetilde{D}^2}], \quad t > 0. \quad (1.5)$$

It is hence of great importance that (cf. eg. [17, Lemma 1.9.1])

- for any differential operator, \widetilde{P} , of order p on $C^\infty(\widetilde{E})$, we have an asymptotic expansion

$$\text{tr}[\widetilde{P} e^{-t\widetilde{D}^2}] \sim_{t \rightarrow 0+} \sum a_j(\widetilde{D}, \widetilde{P}) t^{(j-m-p)/d}. \quad (1.6)$$

Even though it took a long time after the original proof of the Atiyah–Singer Index Theorem [3], [26] until a complete proof could be based on (1.4) and (1.5) (cf. [1], [16]), the heat equation method now seems to be the most powerful tool for extensions of the Index Theorem. Recall that for the important class of twisted Dirac operators, with $\widetilde{E} = \widetilde{S} \oplus \widetilde{F}$, \widetilde{S} a spin bundle on \widetilde{M} , this theorem reads

- $\text{ind } \widetilde{D}_+ = \int_{\widetilde{M}} \hat{A}(\widetilde{M}) \wedge \text{ch } \widetilde{F}$. (1.7)

1.B. Compact manifolds with boundary. In this series of papers, we want to present the extension of the main results quoted above ((1.1), (1.2), (1.3), (1.6), (1.7)) to Dirac type operators on manifolds with boundary.

Though a good part of our results is more or less known, we obtain a conceptually as well as technically transparent derivation of this theory, with considerable simplifications and extensions in most cases. Moreover, the functional analytic approach we have developed lends itself naturally to substantial generalizations, e.g. to situations with non-compact boundaries. The basic inspiration for this approach is, of course, the beautiful work of Atiyah, Patodi, and Singer [2] which we generalize.

To explain our work in greater detail, we consider a compact hypersurface, N , in \widetilde{M} which bounds an open subset, M , of \widetilde{M} . We assume that N is oriented as the boundary of M . We put $E := \widetilde{E} \restriction M$, $D := \widetilde{D} \restriction C^\infty(\overline{M})$. Then D is a first order elliptic differential operator on M , and symmetric in $L^2(E)$ with domain $C_0^\infty(E)$. Recall that D is an operator of *Dirac type* [5, Def. 3.36], [17, Sec. 1.8.2] if D^2 has scalar principal symbol given by the metric tensor, i.e. $\hat{D}(\xi)^2 = |\xi|^2$ for each $\xi \in T^*M$. Note that this class of operators is considerably larger than the class of *Dirac operators associated to a Clifford connection* (or twisted Dirac operators) [23, Sec. II.5], [5, p. 119].

If D is of Dirac type then we obtain in a tubular neighbourhood, U , of N in \widetilde{M} a very simple separation of variables. In fact, U is isometric to $(-\varepsilon_0, \varepsilon_0) \times N$ with metric $dx^2 \oplus g_N(x)$, $x \in (-\varepsilon_0, \varepsilon_0)$, g_N a smooth family of metrics on N , and with $E_N := \widetilde{E} \restriction N$ we obtain the following result.

LEMMA 1.1. *Let D be of Dirac type. As operator in $L^2(E \restriction U)$ with domain $C_0^\infty(E \restriction U)$, D is unitarily equivalent to an operator of the form*

$$\gamma \left(\frac{d}{dx} + A(x) \right) + V(x) \quad (1.8)$$

in $L^2((-\varepsilon_0, \varepsilon_0), L^2(E_N))$ with domain $C_0^\infty((-\varepsilon_0, \varepsilon_0), C^\infty(E_N))$.

Here, $\gamma \in \mathcal{L}(L^2(E_N))$ and $A(x)$ is (the closure of) a symmetric elliptic differential operator on E_N of first order; $\mathcal{D}(A(x)) =: \mathcal{D}$ is independent of x and $A(x)$ depends smoothly on $x \in (-\varepsilon_0, \varepsilon_0)$. Furthermore, $V \in C^\infty((-\varepsilon_0, \varepsilon_0), C^\infty(\text{End}(E_N)))$.

Moreover, the following relations hold:

$$\gamma^* = -\gamma, \quad \gamma^2 = -I, \quad (1.9a)$$

$$\gamma(\mathcal{D}) = \mathcal{D} \text{ and } \gamma A(x) + A(x)\gamma = 0, \quad x \in (-\varepsilon_0, \varepsilon_0). \quad (1.9b)$$

If D is a Dirac operator associated to a Clifford connection, then A can be chosen in such a way that $V = 0$.

This lemma has been widely used for some time, especially in the product case ($g_N(x) \equiv g_N(0)$) where it plays a prominent role in [2]. For non-product

metrics some care is needed to compute $A(x)$ in each specific case, cf. e.g. [17, Sec. 3.10] and [9, Sec. 5].

We will base our analysis on a thorough study of the operator equation (1.8) with the structure properties (1.9); *these properties will be assumed throughout this paper.* This approach is reasonable since the results we are aiming at can be obtained from merging "interior analysis" (to be carried out on \bar{M}) with "boundary" analysis involving the operator (1.8).

The main difference between the analysis of D and \tilde{D} lies, of course, in the fact that D is not essentially self-adjoint on $C_0^\infty(E)$. Moreover, if self-adjoint extensions of D exist, they may differ widely with respect to existence, uniqueness, regularity, and heat trace expansions. It is, therefore, our first task to characterize those self-adjoint extensions which behave nicely with respect to existence, uniqueness, and regularity; this is the purpose of the present paper.

1.C. Results for the model operator. Replacing in (1.8) $L^2(E_N)$ by an arbitrary Hilbert space, H , and $C^\infty(E_N)$ by the domain, H_1 , of a self-adjoint operator A in H , we obtain the model operator

$$D = \gamma \left(\frac{d}{dx} + A \right) \text{ in } \mathcal{H}_0 := L^2(\mathbb{R}_+, H) \text{ with domain } C_0^\infty(\mathbb{R}_+, H_1). \quad (1.10)$$

We will have to deal with variable coefficients but for the purpose of the present introduction we will restrict to the constant coefficient case. Indeed, for most of the problems dealt with in this paper operators with variable coefficients merely appear as perturbations of (1.10), in view of the Kato-Rellich Theorem. Furthermore, since $V(x)$ is a bounded operator, it can be ignored in the discussion of self-adjoint extensions of D .

On $C_0^\infty(\mathbb{R}_+, H_1)$ we clearly have

$$(Df, g)_{\mathcal{H}_0} - (f, Dg)_{\mathcal{H}_0} = \langle f(0), \gamma g(0) \rangle_H. \quad (1.11)$$

Now if D is symmetric on a subspace, \mathcal{D}^0 , of $C_0^\infty(\mathbb{R}_+, H_1)$ then it follows from (1.11) that, with $I - P$ the orthogonal projection onto $\overline{\mathcal{D}^0}$ in H , we have

$$\mathcal{D}^0 \subset \mathcal{D}_P := \{f \in C_0^\infty(\mathbb{R}_+, H_1) \mid Pf(0) = 0\} \quad (1.12a)$$

and

$$I - P \leq \gamma^* P \gamma. \quad (1.12b)$$

Moreover, $D_{P,0} := D \restriction \mathcal{D}_P$ is a symmetric extension of $D \restriction \mathcal{D}^0$. If we assume for a moment that H is of finite dimension then it is readily seen that $D_{P,0}$ is essentially self-adjoint in \mathcal{H}_0 if and only if

$$I - P = \gamma^* P \gamma. \quad (1.13)$$

Indeed, if D_{\max} denotes $(D \restriction C_0^\infty((0, \infty), H_1))^*$ then

$$\mathcal{D}(D_{\max}) \subset H_{1,\text{loc}}(\mathbb{R}_+, H), \quad (1.14)$$

and (1.11) remains valid with D_{\max} in place of D , for $f, g \in \mathcal{D}(D_{\max})$.

An orthogonal projection, P , with (1.13) will be called γ -symmetric; it is easy to see that γ -symmetric projections – and hence self-adjoint extensions of D – exist if and only if

$$\operatorname{sign}(i\gamma \upharpoonright \ker A) = 0. \quad (1.15)$$

As an illustration, note that $i \frac{d}{dx}$ does not admit self-adjoint extensions in $L^2(\mathbb{R}_+)$.

Returning to the general case, we meet the essential difficulty that (1.14) has no reasonable analogue. In particular, elements of $\mathcal{D}(D_{\max})$ do not admit H -valued restrictions to zero. To overcome this obstacle, we imitate the Sobolev scales $H_s(E_N)$ and $H_s(E)$ and their interplay in our abstract setting (which has some tradition in Analysis, cf. eg. [26, Chap. XIII]). $H_s(E_N)$ is replaced by

$$\begin{aligned} H_s &:= H_s(A) \\ &:= \begin{cases} \mathcal{D}(|A|^s), \text{ equipped with the graph norms for } s \geq 0; \\ \text{a suitable dual of } H_{-s}(A), \text{ for } s < 0. \end{cases} \end{aligned} \quad (1.16)$$

We also need

$$H_\infty := H_\infty(A) := \bigcap_{s \in \mathbb{R}} H_s(A);$$

and

$$H_{-\infty} := H_{-\infty}(A) := \bigcup_{s \in \mathbb{R}} H_s(A).$$

Next we introduce, for $n \in \mathbb{Z}_+$,

$$\mathcal{H}_n := \mathcal{H}_n(\mathbb{R}_+, A) := \bigcap_{k=0}^n H_k(\mathbb{R}_+, H_{n-k}(A)), \quad (1.17a)$$

where, for $i, j \in \mathbb{Z}_+$,

$$\begin{aligned} H_i(\mathbb{R}_+, H_j(A)) \\ &:= \left\{ f \in \mathcal{H}_0 \mid \left(\frac{d}{dx} \right)^l f \in L^2(\mathbb{R}_+, H_j(A)), \quad 0 \leq l \leq i \right\}. \end{aligned} \quad (1.17b)$$

By interpolation, we then obtain a scale of Hilbert spaces, $\mathcal{H}_s = \mathcal{H}_s(\mathbb{R}_+, A)$, $s \in \mathbb{R}_+$. (1.17a), (1.17b) also make sense with \mathbb{R} in place of \mathbb{R}_+ ; in this way we obtain the scale $\mathcal{H}_s(\mathbb{R}, A)$. Generalizing the classical Trace Theorem for Sobolev spaces, we have the following result about trace maps which will allow the formulation of boundary conditions.

THEOREM 1.2. *The map*

$$r : C_0^\infty(\mathbb{R}_+, H_\infty) \ni f \longmapsto f(0) \in H_\infty$$

extends by continuity to a map

$$r_s : \mathcal{H}_s \longrightarrow H_{s-1/2}, \quad s > 1/2,$$

and also to a map

$$r^* : \mathcal{D}(D_{\max}) \rightarrow H_{-1/2}.$$

Of course, the loss of regularity under the trace map requires the (continuous) extension of the boundary projections to the space $H_{-1/2}$. To deal with this, we introduce *operators of finite order* on the Hilbert scale $(H_s(A))_{s \in \mathbb{R}}$. Thus, a linear map, $B : H_\infty \rightarrow H_\infty$, is an operator of order $\mu \in \mathbb{R}$ if for each $s \in \mathbb{R}$ there is a constant $C(s)$ such that, for any $x \in H_\infty$,

$$\|Bx\|_{H_s} \leq C(s)\|x\|_{H_{s+\mu}}. \quad (1.18)$$

In particular, B extends to an element of $\mathcal{L}(H_s, H_{s-\mu})$ for all $s \in \mathbb{R}$. The totality of such operators forms the linear space $\text{Op}^\mu(A)$. $\text{Op}^{-\infty}(A) := \bigcap_{\mu \in \mathbb{R}} \text{Op}^\mu(A)$ is called the space of *smoothing operators*.

Thus we will have to require that the boundary projections are elements of $\text{Op}^0(A)$. It follows easily from (1.18) that $\text{Op}^0(A)$ is a *-algebra but it is, in general, not *spectrally invariant* in the sense that $B \in \text{Op}^0(A)$ and B invertible in $\mathcal{L}(H)$ implies $B^{-1} \in \text{Op}^0(A)$. To allow for a minimum of functional constructions, we do need actually even more. We are forced to restrict attention to certain subalgebras, $\Psi^0(A) \subset \text{Op}^0(A)$, satisfying the following two conditions.

$\Psi^0(A)$ is a *-subalgebra of $\text{Op}^0(A)$ containing the smoothing operators and with holomorphic functional calculus;

$\Psi^0(A)$ contains an orthogonal projection $P_+(A)$, satisfying

$$I - P_+(A) = \gamma^* P_+(A) \gamma, \quad P_{(0,\infty)}(A) \leq P_+(A) \leq P_{[0,\infty)}(A). \quad (1.19b)$$

Recall that an algebra, $\mathcal{A} \subset \mathcal{L}(H)$, has holomorphic functional calculus if for $B \in \mathcal{A}$ and f holomorphic in a neighbourhood of $\text{spec } B$ (in $\mathcal{L}(H)$) we have $f(B) \in \mathcal{A}$, where $f(B)$ is defined by the Cauchy integral. Note also that the existence of $P_+(A)$ with (1.19b) is equivalent to (1.15) in the finite dimensional case. In general, if $0 \notin \text{spec}_{\text{ess}} A$ then (1.15) is equivalent to the existence of a spectral projection of A satisfying (1.19b).

Let us illustrate these conditions for the case where A is an elliptic differential operator on $C^\infty(E_N)$ and $N = \partial M$ as in Sec. 1.B. Then we have $H_s(A) \simeq H_s(E_N)$, and a natural choice of the algebra $\Psi^0(A)$ is the algebra of classical pseudodifferential operators on E_N , to be denoted by $\Psi_{\text{cl}}^0(E_N)$. It follows from results of Seeley [31, Thm. 5] that $\Psi_{\text{cl}}^0(E_N)$ has holomorphic functional calculus. Moreover, since $0 \notin \text{spec}_{\text{ess}} A$, we have to verify (1.15) to obtain a spectral projection, $P_+(A)$, of A fulfilling (1.19b); but this is a consequence of the Cobordism Theorem. To see this, we split $H =: H_+ \oplus H_-$ according to the

$\pm i$ -eigenspaces of γ . In view of (1.9),

$$A = \begin{pmatrix} 0 & A_- \\ A_+ & 0 \end{pmatrix}, \quad (1.20)$$

and A_+ is a Fredholm operator with index

$$\text{ind } A_+ = \dim \ker A \cap \ker(\gamma - i) - \dim \ker A \cap \ker(\gamma + i). \quad (1.21)$$

Now it is straightforward to check that there exists an orthogonal projection $P_+(A) \in \text{Op}^0(A)$ with the property (1.19b) if and only if

$$\text{ind } A_+ = 0, \quad (1.22)$$

and this follows from the Cobordism Theorem (cf. the discussion after [12, Cor. 3.6]).

Again from Seeley's work, we deduce that $P_+(A) \in \Psi_{\text{cl}}^0(E_N)$ so (1.19a), (1.19b) are satisfied in a natural way.

Now we are in the position to formulate our results for the model operator. The main theorem of this article reads as follows.

THEOREM 1.3. *Let H be a Hilbert space and A a self-adjoint operator in H . Assume, moreover, that an algebra, $\Psi^0(A) \subset \text{Op}^0(A)$, is given with the properties (1.19a) and (1.19b).*

Then $D_{P,0}$ with domain (1.12a) is essentially self-adjoint in $L^2(\mathbb{R}_+, H)$ for any orthogonal projection $P \in \Psi^0(A)$ with the properties

$$\gamma^* P \gamma = I - P \quad (1.13)$$

and

$$(P, P_+(A)) \text{ is a Fredholm pair.} \quad (1.23)$$

The domain of the closure, D_P , of $D_{P,0}$ is

$$\mathcal{D}(D_P) = \{f \in \mathcal{H}_1(\mathbb{R}_+, A) \mid Pf(0) = 0\}. \quad (1.24)$$

Conversely, if A is discrete then the self-adjointness of $D^* \upharpoonright \mathcal{D}(D_P)$ implies (1.13) and (1.23).

We note that the orthogonal projection $P_-(A) = I - P_+(A) \in \Psi^0(A)$ obviously does not satisfy (1.23). However, we will show in Proposition 4.18 that $D_{P_-(A)}$ is essentially self-adjoint with domain $\mathcal{D}(D_{P_-(A)}) \supsetneq \{f \in \mathcal{H}_1(\mathbb{R}_+, A) \mid Pf(0) = 0\}$ (cf. Proposition 4.15 through 4.19 for a detailed discussion of this phenomenon). Hence the "self-adjointness" in the last statement of the Theorem cannot be replaced by "essentially self-adjoint on \mathcal{D}_P ".

The crucial notion of a Fredholm pair of projections is described in Sec. 3; the proof of Theorem 1.3 takes up Sections 2 to 5; since we do not see a direct way to prove it, we have to interpolate various notions of "regularity" which accounts for the length of our presentation. At the end of Section 5 we give the proof of Theorem 1.3 referring to the several intermediate results.

We can view Theorem 1.3 as the analogue of (1.1) for the model operator. Taking advantage of the self-adjointness of D_P we can try to satisfy (1.2) by setting

$$Q := \int_{|\lambda| \geq 1} \lambda^{-1} dE(\lambda), \quad (1.25)$$

where $E(\lambda) = E_{D_P}(\lambda)$, $\lambda \in \mathbb{R}$, denotes the spectral resolution of D_P .

The regularity result in Theorem 4.13 together with the compactness property expressed in Proposition 2.21 easily yields the following analogue of (1.2) and (1.3).

THEOREM 1.4. *We assume the situation of Theorem 1.3 and, in addition, that A is discrete. For $\phi \in C_0^\infty(\mathbb{R})$ with $\phi = 1$ near 0 we put $Q_\phi := \phi Q$. Then Q_ϕ maps into $\mathcal{D}(D_P)$ and there are compact operators, $K_{r/l,\phi}$, in \mathcal{H} such that*

$$D_P Q_\phi = \phi - K_{r,\phi}, \quad Q_\phi D_P = \phi - K_{l,\phi}. \quad (1.26)$$

Moreover, Q_ϕ is of order -1 and $K_{r/l,\phi}$ of order $-\infty$ with respect to the Sobolev scale $\mathcal{H}_s(\mathbb{R}_+, A)$, $s \in \mathbb{R}_+$.

1.D. Results for manifolds with boundary. It is not difficult to translate Theorems 1.3 and 1.4 into statements on D and the Sobolev scales $H_s(E)$ and $H_s(E_N)$, $s \in \mathbb{R}$. We only need to make Lemma 1.1 somewhat more explicit.

For this, we introduce, on U , the global coordinate

$$x(p) := \text{dist}(p, N), \quad p \in U, \quad (1.27)$$

and denote by

$$\Phi : L^2(E \upharpoonright U) \longrightarrow L^2((-\varepsilon_0, \varepsilon_0), L^2(E_N)) \quad (1.28)$$

the isometry implicit in Lemma 1.1. Then we have the properties

$$\psi \Phi u = \Phi((\psi \circ x)u), \quad \psi \in C^\infty(-\varepsilon_0, \varepsilon_0), u \in L^2(E \upharpoonright U), \quad (1.29a)$$

$$(\Phi u)(0) = u \upharpoonright N, \quad u \in C_0^\infty(E \upharpoonright U), \quad (1.29b)$$

$$\Phi((\psi \circ x)H_s(E)) = \psi \mathcal{H}_s(\mathbb{R}, A), \quad \psi \in C_0^\infty(-\varepsilon_0, \varepsilon_0), s \in \mathbb{R}, \quad (1.29c)$$

which allow us to localize near N and to transfer regularity.

To formulate the boundary conditions, we restrict attention to orthogonal projections in $L^2(E_N)$ which are classical pseudodifferential operators i.e. from now on we choose $\Psi^0(A) = \Psi_{\text{cl}}^0(E_N)$, as indicated above. In the theory of boundary value problems for linear elliptic differential operators, it was observed by Calderón [14] that a prominent role is played by an idempotent, $C^+ \in \Psi_{\text{cl}}^0(E_N)$, with the property that

$$\begin{aligned} C^+(H_s(E_N)) &= N_s(E_N) \\ &:= \{u \in H_s(E_N) \mid u = \tilde{u} \upharpoonright N \text{ for } \tilde{u} \in H_{s+1/2}(E) \text{ with } D\tilde{u} = 0\} \end{aligned} \quad (1.30)$$

for all $s \in \mathbb{R}$; C^+ is called the *Calderón projector* (cf. [30, 28], a comprehensive summary can be found in [19, Appendix]). One checks that

$$C^+ - P_+(A) \in \Psi_{\text{cl}}^{-1}(E_N) \quad (1.31)$$

which explains the importance of the Atiyah–Patodi–Singer boundary condition. In order to obtain boundary conditions which define Fredholm operators (as in (1.2), (1.3)), Seeley introduced the notion of "well-posed" boundary condition [28] which we develop in Section 7 below. Combining the results described so far with Theorem 7.2, we obtain the following optimal version of Seeley's result, as a consequence of our general theory.

THEOREM 1.5. *Let M be a compact manifold with boundary as in Section 1.B and let D be an operator of Dirac type (resp. a first order symmetric elliptic differential operator of the form (1.8)) acting on sections of the hermitian vector bundle E .*

Let $P \in \Psi_{\text{cl}}^0(E_N)$ be an orthogonal projection in $L^2(E_N)$ satisfying (1.13).

Then $D_P := D^ \upharpoonright \mathcal{D}_P := \{f \in H_1(\tilde{E} \upharpoonright \bar{M}) \mid P(f \upharpoonright N) = 0\}$ is self-adjoint in $L^2(E)$ if and only if P is well-posed in the sense of Seeley. This, in turn, is equivalent to the fact that $(P, P_+(A))$ is a Fredholm pair.*

In this case there are a bounded operator, Q , and compact operators, K_r, K_l , in $L^2(E)$ such that Q maps into $\mathcal{D}(D_P)$ and

$$D_P Q = I - K_r, \quad Q D_P = I - K_l.$$

Moreover, with respect to the Sobolev scale $H_s(E)$, $s \in \mathbb{R}_+$, Q is of order -1 and $K_{r/l}$ of order $-\infty$.

The proof of this Theorem is presented at the end of Section 7.

1.E. Further results. Theorem 1.5 is the main application presented here of the results in this paper but, by their abstract character, they apply to more singular situations as well. This will be carried out in part III of this series for covering spaces of compact manifolds with boundary.

Among the material presented here we still have to mention Sec. 6 where we deal with variable coefficients and also, in preparation for the following parts, with the regularity theory of D^2 . Here the reader will find the (fairly easy) arguments necessary to prove the results mentioned above for variable coefficients (i.e. for the case where $g_N(x)$ is not constant near $x = 0$).

The other publications in this series will be devoted to the analogues of the statements (1.6) and (1.7).

In part II, we will develop systematically the index theory of the operator $\gamma\left(\frac{d}{dx} + A(x)\right)$ (with suitable involutions) on finite or infinite intervals, with appropriate boundary conditions. Again, we will simplify and extend various known results but also present some new theorems.

Part III will address index theorems on manifolds with boundary in full generality, based on Theorem 1.5, and we will apply it to the "glueing" of indices. Moreover, we use our techniques to give very simple proofs of various results in index theory like the Cobordism Theorem, or the index theorems of Callias and Ramachandran.

Part IV will derive the heat expansion for the operators described in Theorem 1.5, using only the simple structure of the model operator. In this context, variable coefficients present essential new difficulties. We will pay special attention to the (spectrally defined) determinant of these operators as a function on the Grassmannian of well-posed projections.

Some of the results of this and the forthcoming papers have been announced in [11].

2. Sobolev spaces and operator algebras associated with self-adjoint operators

2.A. The Sobolev scale of an unbounded operator. We consider a Hilbert space, H . We fix a self-adjoint (unbounded) operator A in H and introduce the dense subspace

$$H_\infty := \bigcap_{s \geq 0} \mathcal{D}(|A|^s), \quad (2.1)$$

where \mathcal{D} denotes the domain of an unbounded operator. For $s \in \mathbb{R}$ let $H_s = H_s(A)$ be the completion of H_∞ with respect to the scalar product

$$\langle x, y \rangle_s := \langle (I + A^2)^{s/2} x, (I + A^2)^{s/2} y \rangle, \quad (2.2)$$

such that $H_0 = H$, $H_1 = \mathcal{D}(A)$, and we have embeddings $i_{s',s} : H_{s'} \subset H_s$ of norm at most 1, for $s' > s$. Then $(I + A^2)^{\mu/2}$ induces an isometry $H_s \rightarrow H_{s-\mu}$ for all $s, \mu \in \mathbb{R}$ and we obtain a perfect pairing

$$\begin{aligned} H_{-s} \times H_s &\longrightarrow \mathbb{C}, \\ (x, y) &\longmapsto B_s(x, y) := \langle (I + A^2)^{-s/2} x, (I + A^2)^{s/2} y \rangle_0, \end{aligned} \quad (2.3)$$

with $B_s(x, y) = \langle x, y \rangle_0$ for $x, y \in H_\infty$. In particular

$$|B_s(x, y)| \leq \|x\|_{-s} \|y\|_s. \quad (2.4)$$

If $s \geq 0$ then

$$H_s = \mathcal{D}(|A|^s). \quad (2.5)$$

The natural inclusion map $H_{s'} \hookrightarrow H_s$ is compact if and only if A is *discrete*, i.e. if A has a compact resolvent in H . For $s \in \mathbb{R}$, H_s is a Banach space with strong antidual H_{-s} . H_∞ becomes a Fréchet space under the seminorms $(\|\cdot\|_n)_{n \in \mathbb{Z}}$, with dual space $H_{-\infty} = \cup_{s \in \mathbb{R}} H_s$.

DEFINITION 2.1. A linear map, $T : H_\infty \rightarrow H_\infty$, is called an *operator of order $\mu \in \mathbb{R}$* , if T induces a continuous linear map from H_s to $H_{s-\mu}$, for all $s \in \mathbb{R}$, that is, if for any $s \in \mathbb{R}$ there is a constant $C_s(T)$ such that

$$\|Tx\|_{s-\mu} \leq C_s(T)\|x\|_s, \quad x \in H_\infty. \quad (2.6)$$

T is called *smoothing* or *of order $-\infty$* if it is of order μ for all $\mu \in \mathbb{R}$. We denote the set of all operators of order μ by $\text{Op}^\mu(A)$, $-\infty \leq \mu < \infty$.

PROPOSITION 2.2. (1) *For $T \in \text{Op}^\mu(A)$ let T^* be the Hilbert space adjoint of T considered as an (unbounded) operator in H with domain H_∞ . Then $H_\infty \subset \mathcal{D}(T^*)$ and $T^t := T^* \upharpoonright H_\infty$ is in $\text{Op}^\mu(A)$. In particular, T^* is densely defined (resp. bounded if $\mu \leq 0$).*

(2) *Suppose that $T, T^t : H_\infty \rightarrow H_\infty$ are linear with*

$$\langle Tx, y \rangle = \langle x, T^t y \rangle, \quad x, y \in H_\infty.$$

If T and T^t satisfy (2.6) for some $s_j \geq 0, j \in \mathbb{Z}_+$, with $\lim_{j \rightarrow \infty} s_j = \infty$, then both T and T^t are in $\text{Op}^\mu(A)$.

(3) *Let $T \in \mathcal{L}(H_0)$ with $T(H_s) \subset H_{s-\mu}, T^*(H_s) \subset H_{s-\mu}$ for $s \geq 0$ and some fixed $\mu \leq 0$. Then $T \in \text{Op}^\mu(A)$.*

PROOF. (1) We note first that (2.6) is equivalent to the estimate

$$|\langle Tx, y \rangle| \leq C_s(T)\|x\|_s \|y\|_{\mu-s}, \quad x, y \in H_\infty, s \in \mathbb{R}. \quad (2.6')$$

This implies (1), with $C_s(T^*) = C_{\mu-s}(T)$.

(2) In (2), we have (2.6') for $s_j, j \in \mathbb{Z}_+$, by assumption on T , and from the assumption on T^t we derive (2.6') for $-s_j + \mu, j \in \mathbb{Z}_+$. Hence the assertion follows from complex interpolation.

(3) It follows from the Closed Graph Theorem that T and T^* map H_s continuously into $H_{s-\mu}$, for $s \geq 0$. Then (2) implies the assertion. \square

Note that for any rapidly decreasing Borel function $f : \mathbb{R} \rightarrow \mathbb{R}$ the operator $f(A)$ is smoothing. In particular, $P_0(A)$, the orthogonal projection onto $\ker A$, is smoothing.

COROLLARY 2.3. $\text{Op}^0(A)$ is a $*$ -subalgebra of $\mathcal{L}(H_0)$, the algebra of bounded linear operators on H_0 .

The smoothing operators $\text{Op}^{-\infty}(A)$ form a two-sided $*$ -ideal in $\text{Op}^0(A)$.

PROOF. The product of operators of order 0 is an operator of order 0. Thus $\text{Op}^0(A)$ is an algebra and by the previous Proposition it is a $*$ -algebra. The last statement is obvious. \square

LEMMA 2.4. Let $T \in \text{Op}^\mu(A)$. If $T(H_\infty)$ is finite-dimensional, then T is smoothing.

PROOF. Choose a basis $(f_i)_{i=1}^N$ for $T(H_\infty)$ which is orthonormal in H . We can write, for $x \in H_\infty$,

$$Tx = \sum_{i=1}^N T_i(x) f_i,$$

with $T_i : H_\infty \rightarrow \mathbb{C}$ linear. It follows for $s \in \mathbb{R}$ that

$$|T_i(x)| = |\langle Tx, f_i \rangle| \leq C_s(T) \|x\|_s \|f_i\|_{\mu-s}.$$

But then $T_i(x) = \langle x, e_i \rangle$ for some $e_i \in H_\infty$. \square

DEFINITION 2.5. Slightly more generally, we call a family $(H_s)_{s \in \mathbb{R}}$ ($s \in \mathbb{R}_+$) a *scale of Hilbert spaces* if

- (1) H_s is a Hilbert space for each $s \in \mathbb{R}$ ($s \in \mathbb{R}_+$),
- (2) $H_{s'} \hookrightarrow H_s$ embeds continuously for $s \leq s'$,
- (3) if $s < t, 0 < \theta < 1$, then the complex interpolation space satisfies

$$[H_s, H_t]_\theta = H_{\theta t + (1-\theta)s},$$

- (4) $H_\infty := \bigcap_{s \in \mathbb{R}_+} H_s$ is dense in H_t for each t .

In view of (2.3) the Sobolev scale of an unbounded self-adjoint operator satisfies in addition

- (5) the H_0 -scalar product restricted to H_∞ extends to an antidual pairing between H_s and H_{-s} for all $s \in \mathbb{R}$.

For the complex interpolation method we refer to [32, Sec. 4.2]. A scale $(H_s)_{s \in \mathbb{R}_+}$ satisfying (1)–(4) can be extended to a scale of Hilbert spaces parametrized over \mathbb{R} by defining H_{-s} to be the completion of H_∞ with respect to the norm

$$\|x\|_{-s} := \sup_{y \in H_\infty \setminus \{0\}} \frac{|\langle x, y \rangle|}{\|y\|_s}, \quad s \in \mathbb{R}_+.$$

This family will also satisfy (5). However, the scales of Sobolev spaces on manifolds with boundary usually do not satisfy (5).

Thus, if A is a self-adjoint operator in the Hilbert space H , then $(H_s(A))_{s \in \mathbb{R}}$ is a scale of Hilbert spaces satisfying (5). The converse is almost true: namely, if $(H_s)_{s \in \mathbb{R}}$ is a scale of Hilbert spaces satisfying (5), then for each $N > 0$ there exists a self-adjoint operator A in H_0 with $H_s(A) = H_s$ for $|s| \leq N$ (cf. [25, Sec. 1.2.1]). However, it is not clear whether there exists such an A for all $s \in \mathbb{R}$ simultaneously. For example, we will prove in Corollary 2.20 that $(\mathcal{H}_s(\mathbb{R}_+, A))_{s \in \mathbb{R}_+}$ satisfies (1)–(4), hence it can be extended to a scale of Hilbert spaces parametrized over \mathbb{R} . However, we do not know of a self-adjoint operator B in $L^2(\mathbb{R}_+, H)$ such that $\mathcal{H}_s(\mathbb{R}_+, A) = H_s(B)$ for all $s \geq 0$.

The results of this section have obvious counterparts for a given scale of Hilbert spaces $(H_s)_{s \in \mathbb{R}}$. If the axiom (5) is not satisfied, duality arguments are not possible and one has to restrict attention to $s \geq 0$.

A useful property of an algebra $\mathcal{A} \subset \mathcal{L}(H)$ is its *spectral invariance* by which we mean the assertion

$$T \in \mathcal{A}, T \text{ invertible in } \mathcal{L}(H) \implies T \text{ invertible in } \mathcal{A}. \quad (2.7)$$

A slightly stronger assumption is

$$\mathcal{A} \text{ admits holomorphic functional calculus,} \quad (2.8)$$

by which we mean that for $T \in \mathcal{A}$ and any function f , holomorphic in a neighborhood of $\text{spec } T$, we have $f(T) \in \mathcal{A}$.

We proceed to show that $\text{Op}^0(A)$ is, in general, not spectrally invariant; this will force us to restrict our attention to suitable subalgebras.

PROPOSITION 2.6. *Let A be a discrete operator with eigenvalues $|\mu_0| \leq |\mu_1| \leq |\mu_2| \leq \dots \rightarrow \infty$. Assume that there exists a subsequence $(\mu_{n_k})_{k \in \mathbb{Z}_+}$ satisfying*

$$0 < \lambda_1 \leq \left| \frac{\mu_{n_k}}{\mu_{n_{k+1}}} \right| \leq \lambda_2 < 1 \quad (2.9)$$

for some λ_1, λ_2 .

Then $\text{Op}^0(A)$ is not spectrally invariant in $\mathcal{L}(H_0)$, i.e. there exists an operator $T \in \text{Op}^0(A)$ which is invertible in H_0 but with $T^{-1} \notin \text{Op}^0(A)$.

PROOF. Denote by $(e_n)_{n \in \mathbb{Z}_+}$ an orthonormal basis of H with $Ae_n = \mu_n e_n$. Put for $\xi = \sum_{n=0}^{\infty} \xi_n e_n \in H$

$$K\xi := \sum_{k=0}^{\infty} \xi_{n_{k+1}} e_{n_k}.$$

K is in $\text{Op}^0(A)$ in view of (2.9). Furthermore, we have

$$\|K\|_{H_0 \rightarrow H_0} = 1.$$

Hence for any $0 < \lambda < 1$ the operator $I + \lambda K$ is invertible in H_0 .

Next consider $\xi = (\xi_n)_{n \in \mathbb{Z}_+}$ with

$$\xi_n := \begin{cases} (-1)^k \lambda^{-k}, & n = n_k, \\ 0 & \text{otherwise.} \end{cases}$$

(2.9) implies $\xi \in H_s$ for $s \leq s_0 < 0$ small enough. Since $(I + \lambda K)\xi = 0$ the operator $(I + \lambda K)$ is not invertible in H_s and thus $(I + \lambda K)^{-1} \notin \text{Op}^0(A)$. \square

REMARK 2.7. 1. Gramsch [18, Ex. 6.2] gave the first example of a discrete operator A such that $\text{Op}^0(A)$ is not spectrally invariant. Proposition 2.6 is a generalization of this.

2. We conjecture that for discrete A the algebra $\text{Op}^0(A)$ is never spectrally invariant in $\mathcal{L}(H_0)$.
3. The condition (2.9) is fulfilled if

$$\mu_n \sim Cn^\alpha$$

for some $C, \alpha > 0$. One just takes $n_k := 2^k$. Thus, if A is a self-adjoint elliptic operator on a compact manifold then $\text{Op}^0(A)$ is not spectrally invariant.

2.B. Sobolev spaces on \mathbb{R} and \mathbb{R}_+ .

Let

$$D = \gamma\left(\frac{d}{dx} + A\right) \quad (2.10)$$

as defined in (1.9), (1.10).

Since it will be necessary to distinguish between operators on the whole line \mathbb{R} and on the half line \mathbb{R}_+ we denote by \tilde{D} the operator $\gamma\left(\frac{d}{dx} + A\right)$ acting on $C_0^\infty(\mathbb{R}, H_\infty)$ in $L^2(\mathbb{R}, H)$. This is a symmetric operator in $L^2(\mathbb{R}, H)$ with $\tilde{D}^2 = -\frac{d^2}{dx^2} + A^2$. Furthermore, we put $D_\pm := \tilde{D} \upharpoonright C_0^\infty(\mathbb{R}_\pm^*, H_\infty)$, $\mathbb{R}_\pm^* := \mathbb{R}_\pm \setminus \{0\}$. D_\pm is a symmetric operator in $L^2(\mathbb{R}_\pm, H)$. If no confusion is possible we will write $D := D_+$.

The unique self-adjoint extension of \tilde{D} will be the source of another Sobolev scale which is crucial for our further study.

LEMMA 2.8. *All powers of \tilde{D} are essentially self-adjoint.*

PROOF. The assertion is easy to see for bounded A . But \tilde{D} commutes with the spectral projections of $|A|$ so we can reduce the problem to this case. \square

By a slight abuse of notation, we identify \tilde{D} with its unique self-adjoint extension. Next we define the Sobolev spaces

$$\mathcal{H}_s(\mathbb{R}, A) := H_s(\tilde{D}), \quad s \in \mathbb{R}. \quad (2.11)$$

$\mathcal{H}_s(\mathbb{R}, A)$ is a Hilbert space with norm

$$\|f\|_s^2 = \int_{\mathbb{R}} \|(I + \xi^2 + A^2)^{s/2} \hat{f}(\xi)\|^2 d\xi, \quad (2.12)$$

where

$$\hat{f}(\xi) := \int_{\mathbb{R}} e^{-ix\xi} f(x) dx, \quad d\xi := \frac{1}{2\pi} d\xi.$$

The following maps are continuous:

$$\begin{aligned} \tilde{D}, \frac{d}{dx}, A : \mathcal{H}_s(\mathbb{R}, A) &\longrightarrow \mathcal{H}_{s-1}(\mathbb{R}, A), \\ \gamma, \check{} : \mathcal{H}_s(\mathbb{R}, A) &\longrightarrow \mathcal{H}_s(\mathbb{R}, A), \end{aligned} \quad (2.13)$$

where $(Af)(x) := A(f(x))$, $(\gamma f)(x) := \gamma f(x)$, $\check{f}(x) := f(-x)$.

Furthermore, we put $\mathcal{H}_s(\mathbb{R}_\pm, A) := \{f \upharpoonright \mathbb{R}_\pm \mid f \in \mathcal{H}_s(\mathbb{R}, A)\}$, $s \in \mathbb{R}$, and equip this space with the quotient Hilbert space structure, i.e.

$$\|f\|_s := \inf \{\|\tilde{f}\|_s \mid \tilde{f} \upharpoonright \mathbb{R}_\pm = f\}. \quad (2.14)$$

Clearly, there is a natural restriction map $\mathcal{H}_s(\mathbb{R}, A) \rightarrow \mathcal{H}_s(\mathbb{R}_\pm, A)$ of norm 1. (2.13) also holds with \mathbb{R}_\pm in place of \mathbb{R} , except that $\check{\cdot}$ maps $\mathcal{H}_s(\mathbb{R}_\pm, A)$ continuously into $\mathcal{H}_s(\mathbb{R}_\mp, A)$.

We will prove in Corollary 2.20 below that the family $(\mathcal{H}_s(\mathbb{R}_+, A))_{s \in \mathbb{R}_+}$ is a scale of Hilbert spaces hence, as noted after Definition 2.5, it can be extended to a scale of Hilbert spaces parametrized over \mathbb{R} . We do not claim, however, that $(\mathcal{H}_s(\mathbb{R}_+, A))_{s \in \mathbb{R}}$ is a scale of Hilbert spaces. Although this is conceivable, the family $(\mathcal{H}_s(\mathbb{R}_+, A))_{s \in \mathbb{R}}$ will certainly not satisfy axiom (5). Hence, in the discussion of $\mathcal{H}_s(\mathbb{R}_+, A)$ we will restrict ourselves to the case $s \geq 0$. According to the remark after Definition 2.5 we could extend $(\mathcal{H}_s(\mathbb{R}_+, A))_{s \geq 0}$ to a scale of Hilbert spaces satisfying (5). However, we refrain from doing so for two reasons: first, this definition of Sobolev spaces of negative order would differ from the usual definition on manifolds with boundary [32, Sec. 4.5] and, secondly, integration by parts shows that the operator D would not be of order one for that scale. The spaces $\mathcal{H}_s(\mathbb{R}_+, A)$ for negative s will play no further role in the rest of the paper.

We note that for $s \geq 0$ we have an inclusion $\mathcal{H}_s(\mathbb{R}_{(+)}, A) \subset L^2(\mathbb{R}_{(+)}, H_s)$ of norm less or equal 1. Indeed,

$$\begin{aligned} \int_{\mathbb{R}} \|f(x)\|_{H_s}^2 dx &= \int_{\mathbb{R}} \|\hat{f}(\xi)\|_{H_s}^2 d\xi = \int_{\mathbb{R}} \|(I + A^2)^{s/2} \hat{f}(\xi)\|^2 d\xi \\ &\leq \int_{\mathbb{R}} \|(I + \xi^2 + A^2)^{s/2} \hat{f}(\xi)\|^2 d\xi \\ &= \|f\|_s^2. \end{aligned} \quad (2.15)$$

REMARK 2.9. The Sobolev spaces introduced above can be expressed in terms of standard Sobolev spaces. Namely, we put for a Hilbert space H

$$\begin{aligned} H_k(\mathbb{R}_{(+)}, H) &:= \left\{ f \in L^2(\mathbb{R}_{(+)}, H) \mid \left(\frac{d}{dx}\right)^j f \in L^2(\mathbb{R}_{(+)}, H), 0 \leq j \leq k \right\} \\ &= H_k(\mathbb{R}_{(+)}) \hat{\otimes} H, \end{aligned} \quad (2.16)$$

where $\hat{\otimes}$ denotes the Hilbert space tensor product. Then one infers from (2.13) that for $n \geq 0$

$$\mathcal{H}_n(\mathbb{R}, A) = \bigcap_{k=0}^n H_k(\mathbb{R}, H_{n-k}(A)). \quad (2.17)$$

(cf. [27, p. 8]). (2.17) is also true with \mathbb{R}_+ in place of \mathbb{R} (this is shown in Corollary 2.20 below), this fact, however, is less obvious.

(2.17) can be improved using complex interpolation. We consider Hilbert spaces E, F with self-adjoint operators $B \geq I$ in E and $C \geq I$ in F . We put $E' := \mathcal{D}(B)$, $F' := \mathcal{D}(C)$. Then $B \otimes C$ is a symmetric operator on $H_\infty(B) \otimes H_\infty(C) \subset E \hat{\otimes} F$. This operator is essentially self-adjoint and its unique self-adjoint extension will be denoted by $B \hat{\otimes} C$ (cf. [10]). Since $B \geq I$ we can define the graph norm of B by $\|x\|_B := \|Bx\|_F$. If we define the graph norms of C and $B \hat{\otimes} C$ similarly we see that

$$\mathcal{D}(B \hat{\otimes} C) = E' \hat{\otimes} F'. \quad (2.18)$$

Furthermore, $B \hat{\otimes} I$ and $I \hat{\otimes} C$ are commuting self-adjoint operators with $(B \hat{\otimes} I)(I \hat{\otimes} C) = B \hat{\otimes} C$. Hence we have for any $\theta > 0$

$$(B \hat{\otimes} C)^\theta = B^\theta \hat{\otimes} C^\theta. \quad (2.19)$$

These considerations imply

$$\begin{aligned} [E \hat{\otimes} F, E' \hat{\otimes} F']_\theta &= \mathcal{D}((B \hat{\otimes} C)^\theta) = \mathcal{D}(B^\theta \hat{\otimes} C^\theta) \\ &= \mathcal{D}(B^\theta) \hat{\otimes} \mathcal{D}(C^\theta) = [E, E']_\theta \hat{\otimes} [F, F']_\theta. \end{aligned} \quad (2.20)$$

From the inequality $\frac{1}{2}(b^s + c^s) \leq (b + c)^s \leq 2^s(b^s + c^s)$, for $b, c, s \geq 0$, and the Spectral Theorem we infer

$$\begin{aligned} [E, E']_\theta \hat{\otimes} F \cap E \hat{\otimes} [F, F']_s &= \mathcal{D}(B^s \hat{\otimes} I) \cap \mathcal{D}(I \hat{\otimes} C^s) \\ &= \mathcal{D}((B \hat{\otimes} I + I \hat{\otimes} C)^s) \\ &= [E \hat{\otimes} F, E' \hat{\otimes} F \cap E \hat{\otimes} F']_s. \end{aligned} \quad (2.21)$$

With these preparations we can prove:

PROPOSITION 2.10. *For $s \geq 0$ we have the identities*

$$\bigcap_{0 \leq t \leq s} H_t(\mathbb{R}_{(+)}, H_{s-t}) = H_s(\mathbb{R}_{(+)}, H_0) \cap H_0(\mathbb{R}_{(+)}, H_s), \quad (2.22)$$

and

$$\mathcal{H}_s(\mathbb{R}, A) = H_s(\mathbb{R}, H_0) \cap H_0(\mathbb{R}, H_s). \quad (2.23)$$

(2.23) is to be understood as an equality of Hilbert spaces, i.e. we have norm estimates

$$\begin{aligned} C^{-1}(\|f\|_{H_s(\mathbb{R}, H_0)} + \|f\|_{H_0(\mathbb{R}, H_s)}) \\ \leq \|f\|_{\mathcal{H}_s(\mathbb{R}, A)} \leq C(\|f\|_{H_s(\mathbb{R}, H_0)} + \|f\|_{H_0(\mathbb{R}, H_s)}) \end{aligned} \quad (2.24)$$

for all $f \in \mathcal{H}_s(\mathbb{R}, A)$.

PROOF. We apply (2.18)–(2.21) to the spaces $H_s(\mathbb{R}_{(+)}, H_t) = H_s(\mathbb{R}_{(+)}) \hat{\otimes} H_t$. A consequence of (2.20) is the identity

$$[H_s(\mathbb{R}_{(+)}, H_t), H_{s'}(\mathbb{R}_{(+)}, H_{t'})]_\theta = H_{\theta s' + (1-\theta)s}(\mathbb{R}_{(+)}, H_{\theta t' + (1-\theta)t}), \quad (2.25)$$

in particular

$$[L^2(\mathbb{R}_{(+)}, H_s), H_s(\mathbb{R}_{(+)}, H_0)]_\theta = H_{\theta s}(\mathbb{R}_{(+)}, H_{(1-\theta)s}). \quad (2.26)$$

This implies (2.22). In view of (2.17), (2.21), (2.26), and (2.22) we obtain for $0 \leq s \leq N \in \mathbb{Z}_+$

$$\begin{aligned} \mathcal{H}_s(\mathbb{R}, A) &= [L^2(\mathbb{R}, H_0), \mathcal{H}_N(\mathbb{R}, A)]_{s/N} \\ &= [L^2(\mathbb{R}, H_0), H_N(\mathbb{R}, H_0) \cap H_0(\mathbb{R}, H_N)]_{s/N} \\ &= [L^2(\mathbb{R}, H_0), H_N(\mathbb{R}, H_0)]_{s/N} \cap [L^2(\mathbb{R}, H_0), H_0(\mathbb{R}, H_N)]_{s/N} \\ &= H_s(\mathbb{R}, H_0) \cap H_0(\mathbb{R}, H_s). \end{aligned} \quad (2.27)$$

The first inequality in (2.24) follows from (2.15) and a similar calculation for $\|\cdot\|_{H_s(\mathbb{R}, H_0)}$. Since both norms $\|\cdot\|_{H_s(\mathbb{R}, H_0)}$, $\|\cdot\|_{H_s(\mathbb{R}, H_0)} + \|\cdot\|_{H_0(\mathbb{R}, H_s)}$ are Hilbert space norms on $\mathcal{H}_s(\mathbb{R}, A)$, the first inequality in (2.24) implies the second. \square

The same reasoning would work for \mathbb{R}_+ in place of \mathbb{R} if we knew that $(\mathcal{H}_s(\mathbb{R}_+, A))_{s \geq 0}$ is a scale of Hilbert spaces; this fact is the content of Corollary 2.20.

LEMMA 2.11. *Let $f : \mathbb{R} \times \text{spec } A \rightarrow \mathbb{C}$ be a continuous function. Assume that for fixed $x \in \mathbb{R}$ the function $f(x, \cdot)$ is of polynomial growth.*

(1) *For $u \in H_\infty$, we have*

$$\int_{\mathbb{R}} \|f(x, A)u\|^2 dx \leq \|u\|^2 \sup_{\lambda \in \text{spec } A} \int_{\mathbb{R}} |f(x, \lambda)|^2 dx. \quad (2.28)$$

(2) *For $\varphi \in C_0^\infty(\mathbb{R}, H_\infty)$, the function $x \mapsto f(x, A)\varphi(x)$ is weakly integrable over \mathbb{R} and*

$$\left\| \int_{\mathbb{R}} f(x, A)\varphi(x) dx \right\|^2 \leq \|\varphi\|_{L^2(\mathbb{R}, H)}^2 \sup_{\lambda \in \text{spec } A} \int_{\mathbb{R}} |f(x, \lambda)|^2 dx. \quad (2.29)$$

By continuity, (1) extends to $u \in H$ and (2) extends to $\varphi \in L^2(\mathbb{R}, H)$.

PROOF. $f(x, A)u$ is well-defined since $f(x, \cdot)$ is assumed to be of polynomial growth.

(1) Let $(E(\lambda))_{\lambda \in \mathbb{R}}$ be the spectral resolution of A . Then

$$\begin{aligned} \int_{\mathbb{R}} \|f(x, A)u\|^2 dx &= \int_{\mathbb{R}} \langle f(x, A)u, f(x, A)u \rangle dx \\ &= \int_{\mathbb{R}} \int_{\mathbb{R}} |f(x, \lambda)|^2 d\langle E(\lambda)u, u \rangle dx \\ &\leq \|u\|^2 \sup_{\lambda \in \text{spec } A} \int_{\mathbb{R}} |f(x, \lambda)|^2 dx. \end{aligned}$$

(2) For $u \in H_\infty$ we estimate with (1):

$$\begin{aligned} \int_{\mathbb{R}} |\langle f(x, A)\varphi(x), u \rangle| dx &\leq \int_{\mathbb{R}} \|\varphi(x)\| \|f(x, A)u\| dx \\ &\leq \|\varphi\|_{L^2(\mathbb{R}, H)} \left(\int_{\mathbb{R}} \|f(x, A)u\|^2 dx \right)^{1/2} \\ &\leq \|\varphi\|_{L^2(\mathbb{R}, H)} \|u\| \left(\sup_{\lambda \in \text{spec } A} \int_{\mathbb{R}} |f(x, \lambda)|^2 dx \right)^{1/2}, \end{aligned}$$

which proves both the weak integrability and the estimate. \square

THEOREM 2.12 (Trace Theorem). (1) For $s > 1/2$ the restriction map

$$r : C_0^\infty(\mathbb{R}, H_\infty) \longrightarrow H_\infty, \quad f \longmapsto f(0),$$

induces by continuity bounded linear operators $r : \mathcal{H}_s(\mathbb{R}, A) \rightarrow H_{s-1/2}$ and $r_+ : \mathcal{H}_s(\mathbb{R}_+, A) \rightarrow H_{s-1/2}$.

(2) Let $s > -1/2$. If $f, (I + A^2)^{-1/2}f' \in \mathcal{H}_s(\mathbb{R}, A)$, then we have the estimate

$$\|f(0)\|_{s-1/2} \leq C(\|f\|_s + \|(I + A^2)^{-1/2}f'\|_s).$$

PROOF. (1) For $f \in C_0^\infty(\mathbb{R}, H_\infty)$ we write $f(0) = \int_{\mathbb{R}} \hat{f}(\xi) d\xi$ and estimate with Lemma 2.11:

$$\begin{aligned} \|f(0)\|_{s-1/2}^2 &= \left\| \int_{\mathbb{R}} (I + A^2)^{s/2-1/4} \hat{f}(\xi) d\xi \right\|^2 \\ &= \left\| \int_{\mathbb{R}} (I + A^2)^{s/2-1/4} (\xi^2 + I + A^2)^{-s/2} (\xi^2 + I + A^2)^{s/2} \hat{f}(\xi) d\xi \right\|^2 \\ &\leq \sup_{\lambda > 0} \int_{\mathbb{R}} (1 + \lambda)^{s-1/2} (1 + \lambda + \xi^2)^{-s} d\xi \|f\|_s^2 \\ &= \int_{\mathbb{R}} (1 + \xi^2)^{-s} d\xi \|f\|_s^2. \end{aligned}$$

This proves the assertion for $\mathcal{H}_s(\mathbb{R}, A)$. For $\mathcal{H}_s(\mathbb{R}_+, A)$, it is an immediate consequence of the definition of the quotient norm on $\mathcal{H}_s(\mathbb{R}_+, A)$.

(2) It suffices to prove this estimate for $f \in C_0^\infty(\mathbb{R}, H_\infty)$. By (1) we have

$$\begin{aligned} \|f(0)\|_{s-1/2}^2 &= \|(I + A^2)^{-1/2} f(0)\|_{(s+1)-1/2}^2 \\ &\leq C(s) \int_{\mathbb{R}} \|(I + A^2)^{-1/2}(I + \xi^2 + A^2)^{1/2}(I + \xi^2 + A^2)^{s/2} \hat{f}(\xi)\|^2 d\xi \\ &= C(s) \int_{\mathbb{R}} \|(I + \xi^2 + A^2)^{s/2} \hat{f}(\xi)\|^2 d\xi \\ &\quad + C(s) \int_{\mathbb{R}} \|(I + \xi^2 + A^2)^{s/2}(I + A^2)^{-1/2}\xi \hat{f}(\xi)\|^2 d\xi \\ &= C(s)(\|(I + A^2)^{-1/2} f'\|_s^2 + \|f\|_s^2). \end{aligned} \quad \square$$

The restriction map r is in fact surjective, more precisely:

PROPOSITION 2.13. *Let $u \in H_{s-1/2}$, $\varphi \in H_s(\mathbb{R})$, and put $T := (I + A^2)^{1/2}$. Then the function*

$$f(x) := \varphi(xT)u$$

is in $\mathcal{H}_s(\mathbb{R}, A)$ and

$$\|f\|_s \leq \|\varphi\|_s \|u\|_{s-1/2}.$$

In particular, if $\varphi(0) = 1$ we get a continuous right inverse to the restriction map r by

$$e_\varphi(u)(x) := \varphi(xT)u.$$

Note that this result is valid without any restriction on s .

PROOF. Assume first $\varphi \in \mathcal{S}(\mathbb{R})$ and $u \in H_\infty$. Then $f \in \mathcal{S}(\mathbb{R}, H_\infty)$ and from the spectral theorem we see that

$$\hat{f}(\xi) = T^{-1} \hat{\varphi}(\xi T^{-1}) u.$$

With Lemma 2.11 (1) we obtain

$$\begin{aligned} \|f\|_s^2 &= \int_{\mathbb{R}} \|(\xi^2 + T^2)^{s/2} T^{-1} \hat{\varphi}(\xi T^{-1}) u\|^2 d\xi \\ &\leq \sup_{\lambda > 0} \int_{\mathbb{R}} (\xi^2 + \lambda^2)^s \lambda^{-2s-1} |\hat{\varphi}(\xi/\lambda)|^2 d\xi \|u\|_{s-1/2}^2 \\ &= \|\varphi\|_{H_s(\mathbb{R})}^2 \|u\|_{s-1/2}^2. \end{aligned}$$

Since $\mathcal{S}(\mathbb{R})$ is dense in $H_s(\mathbb{R})$ and H_∞ in $H_{s-1/2}$, we reach the conclusion. \square

COROLLARY 2.14. *Let $s > 1/2 + k$, $k \in \mathbb{Z}_+$. Then the map*

$$r_+^{(k)} : \mathcal{H}_s(\mathbb{R}_+, A) \longrightarrow \bigoplus_{j=0}^k H_{s-1/2-j}, \quad f \longmapsto \bigoplus_{j=0}^k (D^j f)(0),$$

is continuous and surjective. Moreover, there exists a continuous right inverse $e^{(k)}$ to $r_+^{(k)}$ with $e^{(k)} \upharpoonright \bigoplus_{j=0}^k H_\infty$ independent of s .

PROOF. Clearly, by Theorem 2.12 $r_+^{(k)}$ exists and is continuous since

$$D^j : \mathcal{H}_s(\mathbb{R}_+, A) \longrightarrow \mathcal{H}_{s-j}(\mathbb{R}_+, A)$$

is. It remains to construct $e^{(k)}$.

We choose $\varphi \in C_0^\infty(\mathbb{R})$ with $\varphi = 1$ near 0. Then in view of Proposition 2.13 we may choose $e^{(0)} := e_\varphi$; this is independent of $s > 1/2$.

Inductively, we assume that we have constructed $e^{(k)}$. Choose $\varphi \in C_0^\infty(\mathbb{R})$ with

$$\varphi^{(j)}(0) = 0, \quad 0 \leq j \leq k, \quad \varphi^{(k+1)}(0) = 1,$$

and put for $(\xi_0, \dots, \xi_{k+1}) \in \bigoplus_{j=0}^{k+1} H_{s-1/2-j}$, $s > 1/2 + k + 1$,

$$\begin{aligned} e^{(k+1)}(\xi_0, \dots, \xi_{k+1}) \\ := (-\gamma)^{k+1} \varphi(xT) T^{-k-1} (\xi_{k+1} - (D^{k+1} e^{(k)}(\xi_0, \dots, \xi_k))(0)) \\ + e^{(k)}(\xi_0, \dots, \xi_k), \end{aligned}$$

where $T = (I + A^2)^{1/2}$, as in Proposition 2.13. \square

LEMMA 2.15. (1) $\mathcal{D}(D^*) \subset \{f \in L^2(\mathbb{R}_+, H) \mid f' \in L^2(\mathbb{R}_+, H_{-1})\}$, and we have a continuous restriction map $r^* : \mathcal{D}(D^*) \rightarrow H_{-1/2}$, $f \mapsto f(0)$.

(2) For $f_j \in \mathcal{D}(D^*)$, $j = 1, 2$ we have

$$-(D^* f_1, f_2) + (f_1, D^* f_2) = \lim_{\varepsilon \rightarrow 0} \langle \gamma(\varepsilon A + i)^{-1} f_1(0), (\varepsilon A + i)^{-1} f_2(0) \rangle.$$

If $f_j(0) \in H_{1/2}$ for some $j \in \{1, 2\}$ then

$$-(D^* f_1, f_2) + (f_1, D^* f_2) = B_{(-1)^{j+1} 1/2}(\gamma f_1(0), f_2(0)). \quad (2.30)$$

PROOF. (1) For $f \in \mathcal{D}(D^*)$ we have $Af \in L^2(\mathbb{R}_+, H_{-1})$, hence $f' \in L^2(\mathbb{R}_+, H_{-1})$. We apply Theorem 2.12 (2) with $s = 0$ and obtain the estimate

$$\begin{aligned} \|f(0)\|_{-1/2} &\leq C(\|f\| + \|(I + A^2)^{-1/2} f'\|) \\ &\leq C(\|f\| + \|(I + A^2)^{-1/2} D^* f\| + \|(I + A^2)^{-1/2} \gamma Af\|) \\ &\leq C(\|f\| + \|D^* f\|). \end{aligned}$$

(2) For $f \in \mathcal{D}(D^*)$ we put $f_\varepsilon(x) := i(\varepsilon A + i)^{-1} f(x)$. Then we have $f_\varepsilon \in \mathcal{D}(D^*) \cap L^2(\mathbb{R}_+, H_1)$ and $f'_\varepsilon \in L^2(\mathbb{R}_+, H)$. Moreover, $f_\varepsilon \rightarrow f$, $D^* f_\varepsilon = (D^* f)_{-\varepsilon} \rightarrow D^* f$, as

$\varepsilon \rightarrow 0$. Thus, integration by parts gives

$$\begin{aligned} -(D^* f_1, f_2) + (f_1, D^* f_2) &= \lim_{\varepsilon \rightarrow 0} [(D^* f_{1,\varepsilon}, f_{2,\varepsilon}) - (f_{1,\varepsilon}, D^* f_{2,\varepsilon})] \\ &= \lim_{\varepsilon \rightarrow 0} \langle \gamma f_{1,\varepsilon}(0), f_{2,\varepsilon}(0) \rangle \\ &= \lim_{\varepsilon \rightarrow 0} \langle \gamma(\varepsilon A + i)^{-1} f_1(0), (\varepsilon A + i)^{-1} f_2(0) \rangle. \end{aligned}$$

To prove the last assertion we note that if $f_j(0) \in H_{1/2}$ then $\lim_{\varepsilon \rightarrow 0} i(\varepsilon A + i)^{-1} f_j(0) = f_j(0)$ in the $H_{1/2}$ -topology and we reach the conclusion. \square

A similar result holds for D_-^* . This follows immediately from the identity

$$D_-^* \gamma \check{f} = -\gamma(D_+^* f)^\vee. \quad (2.31)$$

A consequence of the previous lemma is the following characterization of the space $\mathcal{H}_n(\mathbb{R}_+, A)$.

PROPOSITION 2.16. *Let $f \in \mathcal{D}((D_+^*)^n)$. Then $f \in \mathcal{H}_n(\mathbb{R}_+, A)$ if and only if there exists a $g \in \mathcal{D}((D_-^*)^n)$ with*

$$(D_-^j g)(0) = (D_+^j f)(0), \quad 0 \leq j \leq n-1. \quad (2.32)$$

PROOF. If $f \in \mathcal{H}_n(\mathbb{R}_+, A)$ then there exists $\tilde{f} \in \mathcal{H}_n(\mathbb{R}, A)$ with $\tilde{f} \upharpoonright \mathbb{R}_+ = f$ and one can take $g := \tilde{f} \upharpoonright \mathbb{R}_-$.

Conversely, assume that $g \in \mathcal{D}((D_-^*)^n)$ satisfies (2.32). Put

$$\tilde{f}(x) := \begin{cases} f(x), & x \geq 0, \\ g(x), & x < 0. \end{cases} \quad (2.33)$$

For $\varphi \in C_0^\infty(\mathbb{R}, H_\infty)$ we find using Lemma 2.15

$$\begin{aligned} |\langle \tilde{f}, \tilde{D}^n \varphi \rangle| &= |\langle (D_+^*)^n f, \varphi \upharpoonright \mathbb{R}_+ \rangle_{L^2(\mathbb{R}_+, H_0)} + \langle (D_-^*)^n g, \varphi \upharpoonright \mathbb{R}_- \rangle_{L^2(\mathbb{R}_-, H_0)}| \\ &\leq C_{\tilde{f}} \|\varphi\|_{L^2(\mathbb{R}, H_0)}, \end{aligned}$$

thus $\tilde{f} \in \mathcal{D}((\tilde{D}^n)^*) = \mathcal{H}_n(\mathbb{R}, A)$ in view of Lemma 2.8. \square

From these facts we get the following regularity result.

COROLLARY 2.17. (1) *For $n \in \mathbb{Z}_+$ we have*

$$\begin{aligned} \mathcal{H}_n(\mathbb{R}_+, A) &= \left\{ f : \mathbb{R}_+ \rightarrow H \mid \begin{array}{l} D^j f \in L^2(\mathbb{R}_+, H), \quad 0 \leq j \leq n, \\ (D^j f)(0) \in H_{n-1/2-j}, \quad 0 \leq j \leq n-1 \end{array} \right\}. \quad (2.34) \end{aligned}$$

(2)

$$\mathcal{H}_{n+1}(\mathbb{R}_+, A) = \{ f \in L^2(\mathbb{R}_+, H) \mid Df \in \mathcal{H}_n(\mathbb{R}_+, A), \quad f(0) \in H_{n+1/2} \}.$$

PROOF. (1) The inclusion " \subset " follows from (2.13) and Corollary 2.14. To prove the converse inclusion we pick f in the right hand side of (2.34) and put

$$g(x) := e^{(n-1)}(f(0), (Df)(0), \dots, (D^{n-1}f)(0))(x), \quad x \leq 0.$$

Now the assertion follows from Proposition 2.16.

(2) follows immediately from (1) by induction. \square

PROPOSITION 2.18. *For a fixed integer N choose $(a_j)_{j=1}^N$ such that*

$$\sum_{j=1}^N (-j)^l a_j = 1, \quad l = 0, 1, \dots, N-1. \quad (2.35)$$

For $f \in C_0^\infty([0, \infty), H_\infty)$ put

$$(E^{(N)} f)(x) := \begin{cases} f(x), & x \geq 0, \\ \sum_{j=1}^N a_j f(-jx), & x < 0. \end{cases}$$

Then $E^{(N)}$ has a continuous extension to a map

$H_s(\mathbb{R}_+, H_0) \cap H_0(\mathbb{R}_+, H_s) \longrightarrow \mathcal{H}_s(\mathbb{R}, A)$, for $s \leq N-1$,
also denoted by $E^{(N)}$.

PROOF. The system (2.35) determines the a_1, \dots, a_N uniquely.

Fix $k \in \mathbb{Z}_+, k \leq N-1$, and $f \in H_k(\mathbb{R}_+, H_0) \cap H_0(\mathbb{R}_+, H_k)$. Then (2.35) implies that the right and left derivatives of $E^{(N)} f$ coincide up to order k at 0. Hence $E^{(N)}$ extends by continuity to a map

$$H_k(\mathbb{R}_+, H_0) \cap H_0(\mathbb{R}_+, H_k) \longrightarrow H_k(\mathbb{R}, H_0) \cap H_0(\mathbb{R}, H_k).$$

The assertion follows from complex interpolation and (2.23). \square

REMARK 2.19. The construction of the extension operator $E^{(N)}$ used here is standard by now (cf. e.g. [32, Sec. 4.4]). Seeley [29] refined the construction of the sequence (a_j) in (2.35) and showed that $E^{(N)}$ can indeed be constructed in such a way that it is independent of N . Such an extension operator extends C^∞ -functions defined in a half space to C^∞ -functions in the whole space. As remarked by Seeley the method of construction of $E^{(N)}$ can be traced back to work of L. Lichtenstein [24] and M.R. Hestenes [20].

COROLLARY 2.20. (1) $(\mathcal{H}_s(\mathbb{R}_+, A))_{s \in \mathbb{R}_+}$ is a scale of Hilbert spaces.

(2) For $s \in \mathbb{R}_+$ we have

$$\mathcal{H}_s(\mathbb{R}_+, A) = H_s(\mathbb{R}_+, H_0) \cap H_0(\mathbb{R}_+, H_s) = \bigcap_{0 \leq t \leq s} H_t(\mathbb{R}_+, H_{s-t}).$$

The norm estimates (2.24) hold with \mathbb{R}_+ in place of \mathbb{R} .

Thus, the operators $E^{(N)}$ defined in Proposition 2.18 have unique continuous extensions

$$E_s^{(N)} : \mathcal{H}_s(\mathbb{R}_+, A) \rightarrow \mathcal{H}_s(\mathbb{R}, A), \quad s \leq N - 1,$$

satisfying $(E^{(N)} f) \upharpoonright \mathbb{R}_+ = f$.

PROOF. (1) Observe first that in view of (2.13) there is a continuous inclusion map

$$\mathcal{H}_s(\mathbb{R}_+, A) \subset H_s(\mathbb{R}_+, H_0) \cap H_0(\mathbb{R}_+, H_s). \quad (2.36)$$

Denote by $R(f) := f \upharpoonright \mathbb{R}_+$ the restriction map onto \mathbb{R}_+ . By definition we have for $s < t$, $\theta \in [0, 1]$

$$\begin{aligned} \mathcal{H}_{\theta t + (1-\theta)s}(\mathbb{R}_+, A) &= R(\mathcal{H}_{\theta t + (1-\theta)s}(\mathbb{R}, A)) \\ &= R([\mathcal{H}_s(\mathbb{R}, A), \mathcal{H}_t(\mathbb{R}, A)]_\theta) \\ &\subset [\mathcal{H}_s(\mathbb{R}_+, A), \mathcal{H}_t(\mathbb{R}_+, A)]_\theta. \end{aligned}$$

To prove the converse let $N \geq t + 1$ be an integer. Then, in view of (2.36) and Proposition 2.18, for $f \in [\mathcal{H}_s(\mathbb{R}_+, A), \mathcal{H}_t(\mathbb{R}_+, A)]_\theta$ we have $E^{(N)}(f) \in [\mathcal{H}_s(\mathbb{R}, A), \mathcal{H}_t(\mathbb{R}, A)]_\theta = \mathcal{H}_{\theta t + (1-\theta)s}(\mathbb{R}, A)$ and thus $f = R(E^{(N)} f) \in \mathcal{H}_{\theta t + (1-\theta)s}(\mathbb{R}_+, A)$. This proves (1).

(2) It suffices to prove the converse inclusion of (2.36). Let $f \in H_s(\mathbb{R}_+, H_0) \cap H_0(\mathbb{R}_+, H_s)$. If $N \geq s + 1$ is an integer then, as before, we have $E^{(N)} f \in \mathcal{H}_s(\mathbb{R}, A)$ and thus $f = R(E^{(N)} f) \in \mathcal{H}_s(\mathbb{R}_+, A)$.

The norm estimates follow from the fact that two comparable Hilbert space norms are equivalent and from the continuity of the inclusion (2.36). \square

We denote by $\mathcal{L}^p(H)$ the von Neumann–Schatten class of p -summable operators in H . A linear map $T : H \rightarrow \tilde{H}$ from the Hilbert space H into the Hilbert space \tilde{H} is in the class \mathcal{L}^p if $T^*T \in \mathcal{L}^{p/2}(H)$; this implies $TT^* \in \mathcal{L}^{p/2}(\tilde{H})$.

PROPOSITION 2.21. *If $(A + i)^{-1}$ is in $\mathcal{L}^p(H)$ (compact), then for any $\varphi \in C_0^\infty(\mathbb{R})$ the map $\mathcal{H}_1(\mathbb{R}_+, A) \hookrightarrow L^2(\mathbb{R}, H)$, $f \mapsto \varphi f$, is of class \mathcal{L}^{p+1} (compact).*

PROOF. W.l.o.g. we may assume $\text{supp } \varphi \subset (0, 1)$. We consider the operator $\tau_0 = -\frac{d^2}{dx^2} + A^2$ on

$$\{f \in C^\infty([0, 1], H_\infty) \mid f(0) = f(1) = 0\}.$$

Since $(A + i)^{-1}$ is compact, the operator A is discrete. By slight abuse of notation let $(e_a)_{a \in \text{spec } A}$ be an orthonormal basis of H with $Ae_a = ae_a$. Clearly, $e_a \in H_\infty$. Then

$$\{\sqrt{2} \sin(n\pi \cdot) \otimes e_a\}_{n \in \mathbb{N}, a \in A} \quad (2.37)$$

is an orthonormal basis of $L^2([0, 1], H)$. Furthermore,

$$\tau_0(\sqrt{2} \sin(n\pi \cdot) \otimes e_a) = (n^2\pi^2 + a^2)\sqrt{2} \sin(n\pi \cdot) \otimes e_a. \quad (2.38)$$

Thus (2.37) is an orthonormal basis of eigenvectors of τ_0 . Hence τ_0 is essentially self-adjoint and $\overline{\tau}_0$ is discrete. This implies that the map $\mathcal{D}(\overline{\tau}_0) \hookrightarrow L^2([0, 1], H)$ is compact.

If $(A + i)^{-1} \in \mathcal{L}^p(H)$ then

$$\begin{aligned} & \sum_{n=1}^{\infty} \sum_{a \in \text{spec } A} (1 + n^2\pi^2 + a^2)^{-p/2-1/2} \\ & \leq C \sum_{a \in \text{spec } A} \int_0^{\infty} (a^2 + t^2 + 1)^{-p/2-1/2} dt \\ & \leq C' \sum_{a \in \text{spec } A} (a^2 + 1)^{-p/2} < \infty, \end{aligned}$$

hence the map $\mathcal{D}(\overline{\tau}_0) \hookrightarrow L^2([0, 1], H)$ is of class $\mathcal{L}^{(p+1)/2}$. Since the map

$$\mathcal{H}_2(\mathbb{R}_+, A) \hookrightarrow L^2(\mathbb{R}, H), f \mapsto \varphi f,$$

factorizes through $\mathcal{D}(\overline{\tau}_0)$ we conclude that $\mathcal{H}_2(\mathbb{R}_+, A) \hookrightarrow L^2(\mathbb{R}, H), f \mapsto \varphi f$, is of class $\mathcal{L}^{(p+1)/2}$, too. Now the assertion follows from interpolation. \square

3. Fredholm pairs

3.A. Fredholm pairs in a Hilbert space. Let H be a Hilbert space. We denote by $\mathcal{P}(H)$ the set of orthogonal projections on H .

DEFINITION 3.1. Let $P, Q \in \mathcal{P}(H)$. The pair (P, Q) is called a Fredholm pair if $Q : \text{im } P \rightarrow \text{im } Q$ is a Fredholm operator. The index of this operator is denoted by $\text{ind}(P, Q)$.

The pair (P, Q) will be called invertible if $Q : \text{im } P \rightarrow \text{im } Q$ is invertible.

We will see below that these definitions are symmetric in P and Q . The notion of a Fredholm pair was introduced by Kato [22, IV.4.1]. Bojarski [6] seems to be the first one who used this concept in the theory of elliptic boundary value problems (cf. also Booss–Wojciechowski [8, Sec. 24],[7]). Recently, the notion was systematically studied by Avron, Seiler, and Simon [4] who apparently were not aware of the earlier literature. The following fact is proved by straightforward calculation [4, Sec. 2]:

PROPOSITION 3.2. *Let $P, Q \in \mathcal{P}(H)$. We put*

$$\begin{aligned} X &:= P - Q, \quad Y := I - P - Q, \\ K &:= 2PQ - P - Q = -(2P - I)X = X(2Q - I). \end{aligned} \tag{3.1}$$

Then

- (1) $X^2 + Y^2 = I$, $XY = -YX$, and X^2 commutes with P and Q .
- (2) $KK^* = K^*K = X^2$, in particular, K is a normal operator. Moreover,

$$\|K\| \leq \|P - Q\|.$$

(3) $Z := I + K$ satisfies $ZQ = PZ = PQ$.

The following proposition gives a useful Fredholm criterion.

PROPOSITION 3.3 ([4, Prop. 3.1]). (P, Q) is a Fredholm pair if and only if

$$\pm 1 \notin \text{spec}_{\text{ess}}(P - Q). \quad (3.2)$$

In this case,

$$\begin{aligned} \ker Q \cap \text{im } P &= \ker(P - Q - I), \\ \text{im } Q \cap \ker P &= \ker(P - Q + I), \end{aligned} \quad (3.3)$$

in particular,

$$\text{ind}(P, Q) = \dim \ker(P - Q - I) - \dim \ker(P - Q + I). \quad (3.4)$$

We see from (3.2) that, indeed, (P, Q) is a Fredholm pair if and only if (Q, P) is.

COROLLARY 3.4. For $P, Q \in \mathcal{P}(H)$ the following statements are equivalent:

- (1) $\|P - Q\| < 1$,
- (2) $\pm 1 \notin \text{spec}(P - Q)$,
- (3) (P, Q) is an invertible pair,
- (4) $l(PQ) = P$, $r(PQ) = Q$ and PQ has closed range (where l and r denote the left and right support, respectively).

PROOF. The equivalence of (1) and (2) follows since $P - Q$ is self-adjoint and $\|P - Q\| \leq 1$. The equivalence of (2) and (3) follows from Proposition 3.3 and the equivalence of (3) and (4) is well-known. \square

Since (1) is symmetric in P, Q this corollary implies that if (P, Q) is invertible then (Q, P) is invertible, too.

REMARK 3.5. We note for future reference that (P, Q) is Fredholm if and only if the operator

$$T := PQ + (I - P)(I - Q) \quad (3.5)$$

is a Fredholm operator. In this case

$$\ker T = \ker T^* = \text{im } Q \cap \ker P \oplus \ker Q \cap \text{im } P, \quad (3.6)$$

hence (P, Q) is an invertible pair if and only if T is invertible. Note that $\text{ind } T$ is always zero.

We will now study deformations of Fredholm pairs.

LEMMA 3.6. *Let $P, Q \in \mathcal{P}(H)$ with $\|P - Q\| < 1$. Then $Z_s := I + sK, 0 \leq s \leq 1$, with K from (3.1), is an invertible and normal operator, $P_s := Z_s Q Z_s^{-1} \in \mathcal{P}(H)$ and*

$$P_1 = P, \quad \|P_s - Q\| < 1, \quad 0 \leq s \leq 1.$$

PROOF. From Proposition 3.2 we infer that K is normal with $\|K\| < 1$, hence Z_s is normal and invertible. Furthermore, $P_1 = ZQZ^{-1} = P$. Moreover,

$$Z_s^* Z_s = I + s(K + K^*) + s^2 X^2 = I + (s^2 - s)X^2 \quad (3.7)$$

commutes with P and Q . Since Z_s is normal we have $P_s \in \mathcal{P}(H)$. We thus also have

$$P_s = U_s Q U_s^* \quad (3.8)$$

with the unitary operator $U_s = Z_s(Z_s Z_s^*)^{-1/2}$.

Since $\|Z_s - I\| \leq \|K\| < 1$ and since Z_s is normal, the spectrum of U_s is contained in $\{z \in \mathbb{C} \mid |z| = 1, |\arg z| \leq \pi/2 - \delta\}$ for some $\delta > 0$. Hence there exists $\varepsilon > 0, 0 < q < 1$ such that for $z \in \text{spec } U_s$ we have

$$|z - \varepsilon| \leq q.$$

Consequently,

$$\|P_s - Q\| = \| [U_s - \varepsilon I, Q] \| \leq q < 1. \quad (3.9)$$

The last estimate uses the fact that for $P \in \mathcal{P}(H)$ and any bounded operator $T \in \mathcal{L}(H)$ we have the estimate

$$\|[P, T]\| \leq \|T\|. \quad (3.10)$$

This follows immediately from

$$[P, T] = PT - TP = PT(I - P) - (I - P)TP. \quad (3.11)$$

The lemma is proved. \square

Next we consider an arbitrary Fredholm pair (P, Q) , $P, Q \in \mathcal{P}(H)$. We put

$$\begin{aligned} P' &:= l(PQ), & Q' &:= r(PQ), \\ P'' &:= P - P', & Q'' &:= Q - Q''. \end{aligned} \quad (3.12)$$

Note that P'' is the orthogonal projection onto $\text{im } P \cap \ker Q$ and Q'' is the orthogonal projection onto $\ker P \cap \text{im } Q$.

Since $PQ = P'Q'$ and since PQ has closed range we infer from Corollary 3.4 that (P', Q') is an invertible pair, hence

$$\|P' - Q'\| < 1. \quad (3.13)$$

Furthermore, by construction

$$P' \leq P, \quad Q' \leq Q. \quad (3.14)$$

Let $U_s = U_s(P', Q')$ be the family of unitaries constructed in the proof of Lemma 3.6. Then

$$P' = U_1 Q' U_1^*. \quad (3.15)$$

Put

$$\tilde{Q} := U_1^* P U_1 = Q' + U_1^* P'' U_1, \quad (3.16)$$

and

$$P_s := U_s \tilde{Q} U_s^*, \quad P'_s := U_s Q' U_s^*, \quad 0 \leq s \leq 1. \quad (3.17)$$

Then one sees that $\|P_s - \tilde{Q}\| < 1$, as in the proof Lemma 3.6, and since $\tilde{Q} - Q'$ is of finite rank, we see that (P_s, Q) , $0 \leq s \leq 1$, is a continuous family of Fredholm pairs with

$$P_0 = \tilde{Q} = Q' + \tilde{Q}'', \quad P_1 = P. \quad (3.18)$$

Thus we have proved the following fact.

LEMMA 3.7. *Let $(P, Q) \in \mathcal{P}(H)$ be a Fredholm pair. Then there is a continuous family of Fredholm pairs (P_s, Q) , $0 \leq s \leq 1$, such that $P_1 = P$ and $P_0 = \tilde{Q} = Q' + \tilde{Q}''$ with a finite rank projection $\tilde{Q}'' \leq (I - Q')$. More precisely, $P_s = U_s \tilde{Q} U_s^*$ where U_s is constructed from P', Q' as in the proof of Lemma 3.6.*

Consider the Fredholm pair (\tilde{Q}, Q) constructed above. We have

$$\begin{aligned} \dim(\ker \tilde{Q} \cap \operatorname{im} Q) &= \dim(\ker \tilde{Q}'' \cap \operatorname{im} Q'') \\ &= \operatorname{rank}(Q'') - \operatorname{rank}(\tilde{Q}'' Q'') \\ \dim(\operatorname{im} \tilde{Q} \cap \ker Q) &= \dim(\operatorname{im} \tilde{Q}'' \cap \ker Q'') \\ &= \operatorname{rank}(\tilde{Q}'') - \operatorname{rank}(\tilde{Q}'' Q''), \end{aligned} \quad (3.19)$$

hence

$$\operatorname{ind}(P, Q) = \operatorname{rank} \tilde{Q}'' - \operatorname{rank} Q''. \quad (3.20)$$

If $\operatorname{ind}(P, Q) = 0$ we can find a path of orthogonal projections of finite rank in the space $(I - Q')(H)$ connecting \tilde{Q}'' and Q'' , and hence we can find a path (P_s, Q) of Fredholm pairs connecting (P, Q) with the pair (Q, Q) .

THEOREM 3.8. *For fixed $Q \in \mathcal{P}(H)$ the connected components of*

$$\{P \in \mathcal{P}(H) \mid (P, Q) \text{ Fredholm}\}$$

are labeled by $\operatorname{ind}(P, Q)$.

More precisely, given $P, P' \in \mathcal{P}(H)$ such that the pairs $(P, Q), (P', Q)$ are Fredholm with the same index then there is a smooth family of unitary operators U_t , $0 \leq t \leq 1$, such that

$$\begin{aligned} U_0 &= I, U_1 P U_1^{-1} = P' \\ (U_t P U_t^{-1}, Q) &\text{ is Fredholm.} \end{aligned}$$

3.B. Fredholm pairs of γ -symmetric projections of order 0. In the discussion of self-adjoint extensions of $D = \gamma(\frac{d}{dx} + A)$ below we will need projections $P \in \mathcal{P}(H)$ which are γ -symmetric in the sense that

$$\gamma P = (I - P)\gamma. \quad (3.21)$$

In particular, we will require the existence of a specific projection with (3.21):

ASSUMPTION 3.9. *There is a spectral projection, $P_+(A)$, of A satisfying (3.21) and, in addition,*

$$1_{[0,\infty)}(A) \geq P_+(A) \geq 1_{(0,\infty)}(A). \quad (3.22)$$

We will write $P_+ := P_+(A)$ if no confusion is possible. Furthermore we abbreviate

$$P_- := P_-(A) := I - P_+(A), \quad (3.23)$$

In view of our basic structural assumptions we easily see the following fact.

PROPOSITION 3.10. *A projection with (3.21) and (3.22) exists if and only if the involution $i\gamma | \ker A$ has signature 0 by which we mean that $\ker(\gamma+i) \cap \ker A \simeq \ker(\gamma-i) \cap A$. A unique such projection exists if and only if $\ker A = 0$.*

Namely, if $i\gamma | \ker A$ has signature 0 we may choose an isometry

$$U : \ker(\gamma + i) \cap \ker A \longrightarrow \ker(\gamma - i) \cap A \quad (3.24)$$

and put

$$\sigma : \ker A \longrightarrow \ker A, \quad \sigma := \begin{pmatrix} 0 & U \\ U^* & 0 \end{pmatrix}. \quad (3.25)$$

Then the orthogonal projection

$$P_+(A, \sigma) := 1_{(0,\infty)}(A) \oplus \frac{I + \sigma}{2} \quad (3.26)$$

satisfies Assumption 3.9 and it is clear that all such projections are in one-one correspondence with unitaries $U : \ker(\gamma + i) \cap \ker A \longrightarrow \ker(\gamma - i) \cap A$.

If $i\gamma$ has signature $\neq 0$ on $\ker A$, we can often remedy this defect by slightly extending H . Namely, w.l.o.g. let V be a Hilbert space with

$$\ker(\gamma + i) \cap \ker A \simeq (\ker(\gamma - i) \cap A) \oplus V. \quad (3.27)$$

If $\dim \ker A < \infty$ then V is finite-dimensional, too. We put

$$\tilde{H} := H \oplus V, \quad \tilde{A} := A \oplus 0, \quad \tilde{\gamma} := \gamma \oplus i. \quad (3.28)$$

In view of (3.27) we have $\ker(\tilde{\gamma} + i) \cap \ker \tilde{A} \simeq \ker(\tilde{\gamma} - i) \cap \ker \tilde{A}$. Hence there exists a unitary operator $\sigma : \ker \tilde{A} \rightarrow \ker \tilde{A}$ with $\sigma^2 = I$, $\sigma\tilde{\gamma} = -\sigma\tilde{\gamma}$, and thus the orthogonal projection

$$P_+(\tilde{A}) := 1_{(0,\infty)}(A) \oplus \frac{I + \sigma}{2} \quad (3.29)$$

satisfies Assumption 3.9 with respect to $\tilde{A}, \tilde{\gamma}$.

DEFINITION 3.11. Let $\mathcal{A} \subset \text{Op}^0(A)$ be an operator algebra. We introduce

$$\mathcal{P}_s(\mathcal{A}) := \left\{ P \in \mathcal{P}(H) \cap \mathcal{A} \mid \begin{array}{l} (P, P_+) \text{ is a Fredholm pair and} \\ P \text{ is } \gamma\text{-symmetric} \end{array} \right\}.$$

Note that for $P \in \mathcal{P}_s(\mathcal{A})$ we have $\gamma(P - P_+) = (P_+ - P)\gamma$, hence

$$\text{ind}(P, P_+) = 0. \quad (3.30)$$

We want to derive the analogue of Theorem 3.8 for $\mathcal{P}_s(\mathcal{A})$. For this to work we need an additional structural property of the algebra in question. Thus from now on we consider algebras, $\Psi^0(A) \subset \text{Op}^0(A)$, with the following properties (cf. (1.19) in the introduction):

$\Psi^0(A)$ is a $*$ -subalgebra of $\text{Op}^0(A)$ containing the smoothing operators and with holomorphic functional calculus; (3.31a)

$\Psi^0(A)$ contains an orthogonal projection P_+ with the properties stated in Assumption 3.9. (3.31b)

Assuming (3.31a), in view of Proposition 3.10 property (3.31b) is satisfied if we can find $U \in \Psi^0(A)$ as in (3.24), since all finite spectral projections of A are smoothing.

Then the above construction goes through to yield the following result.

THEOREM 3.12. $\mathcal{P}_s(\Psi^0(A))$ is path connected. More precisely, given $P, Q \in \mathcal{P}_s(\Psi^0(A))$ there is a path $P_t \in \mathcal{P}_s(\Psi^0(A)), 0 \leq t \leq 1$, connecting P and Q such that $t \mapsto P_t$ is smooth for all H_s -norms. P_t can be chosen of the form $P_t = U_t P_0 U_t^{-1}$ where U_t , for $0 \leq t \leq 1$, is a smooth family of unitaries in $\Psi^0(A)$ satisfying

$$\begin{aligned} U_0 &= I, U_t \gamma = \gamma U_t, \\ \text{and } t \mapsto U_t &\text{ is smooth for all } H_s\text{-norms.} \end{aligned}$$

PROOF. Let $X = P - P_+, Y = I - P - P_+, K = 2PP_+ - P - P_+$ (cf. Proposition 3.2). Note the relations

$$\begin{aligned} \gamma X &= -X\gamma, & \gamma Y &= -Y\gamma \\ \gamma K &= K\gamma, & X, Y, K \in \Psi^0(A). \end{aligned} \quad (3.32)$$

Furthermore, $Z_s = I + sK \in \Psi^0(A)$ and commutes with γ . Thus if $\|P - P_+\| < 1$ then in view of Lemma 3.6 and (3.8)

$$P_s = Z_s P_+ Z_s^{-1} = U_s P_+ U_s^*, \quad U_s = Z_s (Z_s Z_s^*)^{-1/2} \quad (3.33)$$

is the desired family of projections in $\mathcal{P}_s(\Psi^0(A))$ connecting P and P_+ . Here, we only used the spectral invariance of $\Psi^0(A)$.

Next we consider a general $P \in \mathcal{P}_s(\Psi^0(A))$. To show that there is a path from P to P_+ having the desired properties we repeat the construction (3.12)–(3.18). The invariance under holomorphic functional calculus of $\Psi^0(A)$ implies $P'' \in \Psi^0(A)$ and thus $P' \in \Psi^0(A)$. To see this note that P'' is the orthogonal projection onto $\text{im } P \cap \ker P_+ = \ker(P - P_+ - I)$ and $0 \notin \text{spec}_{\text{ess}}(P - P_+ - I)$ by Proposition 3.3. Thus P'' is an analytic function of $P - P_+ - I \in \Psi^0(A)$. Analogously, we have $P'_+, P''_+ \in \Psi^0(A)$.

However, since $P' \leq P$, it is γ -symmetric only if $P'' = 0$, hence $P' \notin \mathcal{P}_s(\Psi^0(A))$ if $P'' \neq 0$. We next show that $P' + P''_+ \in \mathcal{P}_s(\Psi^0(A))$.

P''_+ is the orthogonal projection onto $\text{im } P_+ \cap \ker P = \ker(I - P_+) \cap \text{im}(I - P)$, thus by symmetry

$$\gamma P'' \gamma^* = P''_+. \quad (3.34)$$

Since $\text{im } P''_+ \perp \text{im } P'$, $P' + P''_+ \in \Psi^0(A)$ is an orthogonal projection and, by (3.34), it is γ -symmetric. Furthermore, by (3.13)

$$\|(P' + P''_+) - P_+\| = \|P' - P'_+\| < 1, \quad (3.35)$$

thus $(P' + P''_+, P_+)$ is an invertible pair. Thus by the first part of this proof, there is a path from $P' + P''_+$ to P_+ in $\mathcal{P}_s(\Psi^0(A))$ with the desired properties.

As similar argument as in the proof of Theorem 3.8 now shows that there also is such a path from $P' + P''_+$ to P . \square

4. Regularity for the model operator

In this section we study the operator $D = D_+$ and the associated boundary value problems on \mathbb{R}_+ .

In view of (2.30) it is natural to consider, for an orthogonal projection $P \in \text{Op}^0(A)$, the operator D_P given by

$$\begin{aligned} \mathcal{D}(D_P) &:= \{u \in \mathcal{H}_1(\mathbb{R}_+, A) \mid Pu(0) = 0\}, \\ D_P &:= D^* \upharpoonright \mathcal{D}(D_P). \end{aligned} \quad (4.1)$$

Since P is of order zero and, by Lemma 2.15, $u(0) \in H_{-1/2}$ for $u \in \mathcal{D}(D^*)$ we have a natural extension of D_P (which we denote by $D_{P,\max}$) given by

$$\begin{aligned} \mathcal{D}(D_{P,\max}) &:= \{u \in \mathcal{D}(D^*) \mid Pu(0) = 0\}, \\ D_{P,\max} &:= D^* \upharpoonright \mathcal{D}(D_{P,\max}). \end{aligned} \quad (4.2)$$

We are mainly interested in those projections which render D_P self-adjoint. To characterize them, we prepare two results.

- PROPOSITION 4.1.** (1) D_P is symmetric if and only if $I - P \leq \gamma P \gamma^*$.
(2) Let P_1, P_2 be orthogonal projections in $\text{Op}^0(A)$. Then $P_1 \leq P_2$ ($P_1 \neq P_2$) implies $D_{P_2} \subset D_{P_1}$ ($D_{P_1} \neq D_{P_2}$).

PROOF. (1) By Lemma 2.15, we have for $u, v \in \mathcal{D}(D_P)$

$$(-D_P u, v) + (u, D_P v) = \langle \gamma u(0), v(0) \rangle.$$

Thus D_P is symmetric if and only if for all $\xi, \eta \in \ker(P \restriction H_{1/2})$

$$\langle \gamma \xi, \eta \rangle = 0,$$

the "only if" part following from Proposition 2.13. But this is easily seen to be equivalent to $I - P \leq \gamma P \gamma^*$.

(2) $P_1 \leq P_2$ implies $D_{P_2} \subset D_{P_1}$. If $P_1 \leq P_2, P_1 \neq P_2$, then we choose $\xi \in (H_{1/2} \setminus \{0\}) \cap (\ker P_2 \setminus \ker P_1)$. By Proposition 2.13, we can find $f \in \mathcal{H}_1(\mathbb{R}_+, A)$ with $f(0) = \xi$. Then $f \in \mathcal{D}(D_{P_2}) \setminus \mathcal{D}(D_{P_1})$. \square

We will show in Theorem 4.3 below that if $(I - P) \not\leq \gamma^* P \gamma$ then D_P is not self-adjoint.

We abbreviate for $a \in \mathbb{R}$

$$\begin{aligned} P_{<a} &:= 1_{(-\infty, a)}(A), & P_{\leq a} &:= 1_{(-\infty, a]}(A), \\ P_{>a} &:= I - P_{\leq a}, & P_{\geq a} &:= I - P_{<a}. \end{aligned} \tag{4.3}$$

LEMMA 4.2. Let $r^* : \mathcal{D}(D^*) \rightarrow H_{-1/2}$ be the restriction map from Lemma 2.15. We have

$$r^*(\mathcal{D}(D^*)) = P_{>0}(H_{-1/2}) \oplus P_{\leq 0}(H_{1/2}), \tag{4.4a}$$

in particular

$$r^*(\mathcal{D}(D_{P_{>0,\max}})) = P_{\leq 0}(H_{1/2}) \subset H_{1/2}. \tag{4.4b}$$

PROOF. We choose $\chi \in C_0^\infty(\mathbb{R})$, $\chi = 1$ near 0, and put for $f \in \mathcal{D}(D_{P_{>0,\max}})$

$$g(x) := \chi(x)e^{-Ax}f(0), \quad x \leq 0. \tag{4.5}$$

Then $g \in \mathcal{D}(D_-)^*, g(0) = f(0)$, so from Proposition 2.16 we infer $f \in \mathcal{H}_1(\mathbb{R}_+, A)$ and hence $f(0) \in H_{1/2}$. This proves $r^*(\mathcal{D}(D_{P_{>0,\max}})) \subset H_{1/2}$.

To prove (4.4a) let $f \in \mathcal{D}(D^*)$. Then by Lemma 2.15 we have $f(0) \in H_{-1/2}$. Moreover, $x \mapsto P_{\leq 0}f(x)$ lies in $\mathcal{D}(D_{P_{>0,\max}})$ and hence by the first part of the proof we have $P_{\leq 0}f(0) \in H_{1/2}$.

Conversely, let $\xi \in P_{>0}(H_{-1/2}), \eta \in P_{\leq 0}(H_{1/2})$ be given. By Proposition 2.13 there exists $f \in \mathcal{H}_1(\mathbb{R}_+, A)$ with $f(0) = \eta$. Since $P_{\leq 0}\xi = 0$ we see that (4.5), with ξ in place of $f(0)$, defines, for $x > 0$, a function g in $\mathcal{D}(D^*)$ with $g(0) = \xi$. Thus $\xi + \eta = r^*(f + g)$ and we reach the conclusion. \square

Now we present the main result of this section.

THEOREM 4.3. *Let $P \in \text{Op}^0(A)$ be an orthogonal projection.*

- (1) $D_P^* = D_{\gamma^*(I-P)\gamma,\max}$.
- (2) *The following statements are equivalent:*
 - (i) $D_P = D_{P,\max}$. (4.6a)
 - (ii) $r^*(\mathcal{D}(D_{P,\max})) \subset H_{1/2}$. (4.6b)
 - (iii) *If $\xi \in H_{-1/2}$ satisfies $P\xi = 0$ and $P_{<0}\xi \in H_{1/2}$, then also $\xi \in H_{1/2}$.* (4.6c)

PROOF. (1) For $f \in \mathcal{D}(D_{\gamma^*(I-P)\gamma,\max})$ and $g \in \mathcal{D}(D_P)$ we have by Lemma 2.15 (2)

$$\begin{aligned} -(D^*f, g) + (f, D^*g) &= B_{1/2}(\gamma f(0), g(0)) \\ &= B_{1/2}(P\gamma f(0), (I - P)g(0)) = 0, \end{aligned} \quad (4.7)$$

since the last written sesquilinear form vanishes identically on $H_\infty \times H_\infty$ and extends to $H_{-1/2} \times H_{1/2}$ by continuity. Hence $D_{\gamma^*(I-P)\gamma,\max} \subset D_P^*$.

To prove $D_P^* \subset D_{\gamma^*(I-P)\gamma,\max}$ we consider $f \in \mathcal{D}(D_P^*)$. Since $D_P^* \subset D^*$, (4.7) gives for all $g \in \mathcal{D}(D_P)$

$$0 = B_{1/2}(\gamma f(0), g(0)) = B_{1/2}((I - P)\gamma f(0), g(0)). \quad (4.8)$$

By Corollary 2.14, this implies $\gamma^*(I - P)\gamma f(0) = 0$ and hence

$$f \in \mathcal{D}(D_{\gamma^*(I-P)\gamma,\max}).$$

(2) (i) \Rightarrow (ii): This follows immediately from the definition of D_P and the Trace Theorem 2.12.

(ii) \Rightarrow (i): In view of Corollary 2.17 (1), (ii) implies that $\mathcal{D}(D_{P,\max}) \subset \mathcal{H}_1(\mathbb{R}_+, A)$ and thus (i).

(ii) \Rightarrow (iii): Let $\xi \in H_{-1/2}$, $P\xi = 0$, $P_{<0}\xi \in H_{1/2}$. Then, in view of Lemma 4.2, $\xi \in r^*(\mathcal{D}(D^*))$; hence there exists $f \in \mathcal{D}(D^*)$ with $f(0) = \xi$. Since $P\xi = 0$ we have $f \in \mathcal{D}(D_{P,\max})$ and thus $\xi = f(0) \in H_{1/2}$.

(iii) \Rightarrow (ii): If $f \in \mathcal{D}(D_{P,\max})$ then, again by Lemma 4.2, we have $f(0) \in H_{-1/2}$, and $P_{<0}f(0) \in H_{1/2}$; since $Pf(0) = 0$, (iii) implies $f(0) \in H_{1/2}$. \square

Theorem 4.3 motivates the following terminology.

DEFINITION 4.4. P is called *regular* (with respect to D), if one of the equivalent conditions (4.6) is fulfilled.

Inductively, we call P *n-regular* (with respect to D) for $n \geq 2$, if P is $(n-1)$ -regular and

$$\mathcal{D}(D_P^n) \subset \mathcal{H}_n(\mathbb{R}_+, A).$$

Note that, for a regular projection, the restriction map $r^* : \mathcal{D}(D_P) \rightarrow H_{1/2}$ is continuous.

REMARK 4.5. One should note that n -regularity is a relative notion, i.e. in view of (4.6c) it depends on P_+ . More precisely, we should therefore refer to the n -regular pair (P, P_+) . However, since A is fixed once and for all we avoid this notion for simplicity. Referring to the pair (P, P_+) cannot be avoided, however, in the case of “Fredholmness” (Definition 3.1) and “ellipticity” (Definition 4.9). The reason is that the pair (P, P_+) can be Fredholm (resp. elliptic) without P having this property.

We note two consequences of Theorem 4.3.

COROLLARY 4.6. *Let $P \in \text{Op}^0(A)$ be an orthogonal projection. Then D_P is self-adjoint if and only if P is regular and γ -symmetric (in the sense of (3.21)).*

COROLLARY 4.7. *Let $P \in \text{Op}^0(A)$ be an orthogonal projection. Then*

$$\mathcal{D} := \{u \in C_0^\infty([0, \infty), H_\infty) \mid Pu(0) = 0\}$$

is a core for D_P .

PROOF. For the moment we put $T := D_P \upharpoonright \mathcal{D}$. Certainly, we have $D \subset T \subset D_P$ and thus $D_P^* \subset T^* \subset D^*$. We will show $T^* \subset D_P^* = D_{\gamma^*(I-P)\gamma, \max}$; then $T^* = D_P^*$ and hence $\overline{T} = T^{**} = D_P^{**} = \overline{D_P}$.

For $f \in \mathcal{D}(T^*)$ and $g \in \mathcal{D}(T)$ we find as in the previous proof

$$B_{1/2}(\gamma f(0), g(0)) = 0.$$

Since $\ker \gamma^*(I - P)\gamma \cap H_\infty$ is dense in $\ker \gamma^*(I - P)\gamma$ this implies $\gamma^*(I - P)\gamma f(0) = 0$ and thus $f \in \mathcal{D}(D_{\gamma^*(I-P)\gamma, \max}) = \mathcal{D}(D_P^*)$. \square

We add a few comments on why the equivalent conditions of Theorem 4.3 should be referred to as “regularity”.

Consider the equation

$$D^*f = g \tag{4.9}$$

with $f, g \in L^2(\mathbb{R}_+, H)$. In general, (4.9) does not imply $f \in \mathcal{H}_1(\mathbb{R}_+, A)$, but Theorem 4.3 tells us that

$$\begin{aligned} D^*f &= g, \quad f, g \in L^2(\mathbb{R}_+, H), \\ Pf(0) &= 0 \end{aligned} \tag{4.10}$$

implies $f \in \mathcal{H}_1(\mathbb{R}_+, A)$ if and only if P is regular. n -regularity can be characterized similarly:

PROPOSITION 4.8. *An orthogonal projection $P \in \text{Op}^0(A)$ is n -regular if and only if the relations*

$$\begin{aligned} D^*f &= g \in \mathcal{H}_k(\mathbb{R}_+, A), \quad f \in L^2(\mathbb{R}_+, H), \\ Pf(0) &= 0, \end{aligned} \tag{4.11}$$

imply $f \in \mathcal{H}_{k+1}(\mathbb{R}_+, A)$, for $k \in \mathbb{Z}_+, 0 \leq k \leq n - 1$.

PROOF. Let P be a n -regular projection and consider the relations (4.11) for some k . Put

$$f_1 := f - e^{(k+1)}(0, (Df)(0), \dots, (D^k f)(0)),$$

where $e^{(k+1)}$ is defined in Corollary 2.14.

f_1 is well-defined since $Df \in \mathcal{H}_k(\mathbb{R}_+, A)$. By construction, $f_1 \in \mathcal{D}(D_P^{k+1})$, which is contained in $\mathcal{H}_{k+1}(\mathbb{R}_+, A)$ since P is n -regular. But since $(D^j f)(0) \in H_{k+1/2-j}$, $1 \leq j \leq k$, we have $e^{(k+1)}(0, (Df)(0), \dots, (D^k f)(0)) \in \mathcal{H}_{k+1}(\mathbb{R}_+, A)$ hence $f \in \mathcal{H}_{k+1}(\mathbb{R}_+, A)$.

Conversely, if (4.11) implies $f \in \mathcal{H}_{k+1}(\mathbb{R}_+, A)$, $0 \leq k \leq n-1$, then obviously $\mathcal{D}(D_P^k) \subset \mathcal{H}_k(\mathbb{R}_+, A)$, $1 \leq k \leq n$, and hence P is n -regular. \square

Of considerable importance are those projections which are n -regular for all $n \in \mathbb{Z}_+$.

DEFINITION 4.9. Let $P \in \text{Op}^0(A)$ be an orthogonal projection. The pair (P, P_+) is called *elliptic* if P is n -regular for all $n \in \mathbb{Z}_+$.

In Proposition 5.3 we will express ellipticity completely in terms of the orthogonal projections P, P_+ such that it could equally well be defined for any pair (P, Q) of orthogonal projections in $\text{Op}^0(A)$.

Now consider an orthogonal projection $P \in \text{Op}^0(A)$ such that (P, P_+) is elliptic. Can $k \in \mathbb{Z}_+$ in Proposition 4.8 be replaced by any nonnegative real number? We are going to show that if D_P is self-adjoint, then this is indeed true and follows from complex interpolation. But since we will need the argument again below we state the result in the more general framework of scales of Hilbert spaces:

DEFINITION 4.10. Let $(H_s)_{s \in \mathbb{R}_{(+)}}$ be a scale of Hilbert spaces and let $B \in \text{Op}^\mu := \text{Op}^\mu((H_s)_{s \in \mathbb{R}_{(+)}})$. B is called *regular at $s_0 \geq 0$* if

$$u \in H_0, Bu \in H_{s_0} \text{ or } B^t u \in H_{s_0} \implies u \in H_{s_0+\mu}. \quad (4.12)$$

If the scale is parametrized over \mathbb{R} and satisfies axiom (5) (cf. Definition 2.5), then B is called *elliptic* if for all $s \in \mathbb{R}$ we have

$$u \in H_{-\infty}, Bu \in H_s \text{ or } B^t u \in H_s \implies u \in H_{s+\mu}. \quad (4.13)$$

For the definition of B^t see Proposition 2.2 (1).

PROPOSITION 4.11. Let $(H_s)_{s \in \mathbb{R}}$ be a scale of Hilbert spaces satisfying axiom (5). Let $B \in \text{Op}^\mu$ for some $\mu \geq 1$ and assume that B is self-adjoint as an operator in H_0 . Then the following statements are equivalent:

- (i) B is regular at all $n \in \mathbb{Z}_+$,
- (ii) $(B - i)^{-1} \in \text{Op}^{-\mu}$,
- (iii) B is elliptic.

If we have only $\mu > 0$ then (ii) and (iii) are still equivalent.

- REMARK 4.12. 1. If one and hence all of the three equivalent conditions are fulfilled, then we infer in particular that the domain of B , considered as a self-adjoint operator in H_0 , is H_μ .
2. Let $B \in \text{Op}^\mu$, $\mu \geq 0$, be symmetric, i.e. $\langle Bu, v \rangle = \langle u, Bv \rangle$ for $u, v \in H_\infty$. If B is regular at 0, then $B : H_1 \rightarrow H_0$ is a self-adjoint operator in H_0 . Since H_∞ is dense in H_1 , $B \upharpoonright H_\infty$ is essentially self-adjoint.
3. If $H_s = H_s(A)$ then the operators A and $|A|^\alpha$, $\alpha \geq 0$, are elliptic. This follows from the previous proposition and the fact that for $s \in \mathbb{R}$ the operators

$$(I + |A|^2)^{-s+1/2}(A - i)^{-1}(I + |A|^2)^s,$$

$$(I + |A|^2)^{-s+\alpha/2}(|A|^\alpha - i)^{-1}(I + |A|^2)^s$$

are bounded in H_0 . The latter follows from the Spectral Theorem.

PROOF. (iii) \Rightarrow (i) is clear.

(i) \Rightarrow (ii): Let $v \in H_n$, $n \in \mathbb{Z}_+$. Then $u := (B \pm i)^{-1}v \in H_0$ and thus

$$Bu = v \mp iu \in H_0.$$

Since $\mu \geq 1$, the regularity at 0 implies $u \in H_1$ and iterating this argument shows $v \pm iu \in H_n$. Then (i) implies $u \in H_{n+\mu}$.

We have proved that $(B \pm i)^{-1}$ maps H_n into $H_{n+\mu}$ for all $n \in \mathbb{Z}_+$. Now (ii) follows from Proposition 2.2.

(ii) \Rightarrow (iii): We note first that $(B \pm i)^{-1}$ maps H_∞ bijectively onto $H_{-\infty}$ with inverse $B \pm i$. Namely, since B is self-adjoint, $(B \pm i)(B \pm i)^{-1} \upharpoonright H_0 = \text{id}_{H_0}$ and $(B \pm i)^{-1}(B \pm i) \upharpoonright H_1 = \text{id}_{H_1}$. Since $H_\infty \subset H_1 \subset H_0$ and $(B \pm i)^{\pm 1}$ leaves H_∞ invariant, we have $(B \pm i)^{\pm 1}(B \mp i)^{\mp 1} \upharpoonright H_\infty = \text{id}_{H_\infty}$ and by duality these identities also hold for $H_{-\infty}$.

Let $u \in H_{-\infty}$ and $v := Bu \in H_s$. We have $u \in H_t$ for some $t \in \mathbb{R}$ and

$$u = (B - i)^{-1}v - i(B - i)^{-1}u \in H_{\min(s,t)+\mu},$$

from (ii). Iterating this argument we find $u \in H_{s+\mu}$. \square

Now assume that D_P is self-adjoint. Then the previous result does not apply directly to D_P since D_P is not an operator of order 1 with respect to the scale $(\mathcal{H}_s(\mathbb{R}_+, A))_{s \in \mathbb{R}_+}$: the problem is that D_P is not defined on $\mathcal{H}_\infty(\mathbb{R}_+, A)$. However, the proof of the previous result shows that the following slight modification of Proposition 4.11 is true.

PROPOSITION 4.11'. Let $(H_s)_{s \in \mathbb{R}_+}$ be a scale of Hilbert spaces and let $B \in \text{Op}^\mu$, $\mu \geq 1$. Let \tilde{B} be a self-adjoint operator in H_0 with $B \upharpoonright \mathcal{D}(\tilde{B}) = \tilde{B}$. Then the following statements are equivalent:

- (i) For all $n \in \mathbb{Z}_+$: $u \in \mathcal{D}(\tilde{B})$, $Bu \in H_n \implies u \in H_{n+\mu}$,
- (ii) $(\tilde{B} - i)^{-1} \in \text{Op}^{-\mu}$,

(iii) for all $s \in \mathbb{R}_+$: $u \in \mathcal{D}(\tilde{B})$, $Bu \in H_s \implies u \in H_{s+\mu}$.

In view of (2.13), D may be considered as an operator of order 1 with respect to the scale of Hilbert spaces $(\mathcal{H}_s(\mathbb{R}_+, A))_{s \in \mathbb{R}_+}$. Then Proposition 4.11' applies to D_P . Summing up we have proved the following regularity theorem.

THEOREM 4.13 (Regularity Theorem). *Let $P \in \text{Op}^0(A)$ be a γ -symmetric orthogonal projection. The pair (P, P_+) is elliptic if and only if for all $s \in \mathbb{R}_+$ the relations*

$$\begin{aligned} D^*f = g &\in \mathcal{H}_s(\mathbb{R}_+, A), \quad f \in L^2(\mathbb{R}_+, H), \\ Pf(0) &= 0, \end{aligned} \tag{4.14}$$

imply $f \in \mathcal{H}_{s+1}(\mathbb{R}_+, A)$.

PROOF. The "if" part follows from Proposition 4.8. For the "only if" part it remains to note that D_P is self-adjoint, in view of Corollary 4.6. Hence the previous discussion applies. \square

The Regularity Theorem allows to improve Corollary 2.17 (2).

PROPOSITION 4.14. *For all $s \geq 0$ we have*

$$\begin{aligned} \mathcal{H}_{s+1}(\mathbb{R}_+, A) \\ = \{f \in L^2(\mathbb{R}_+, H) \mid Df \in \mathcal{H}_s(\mathbb{R}_+, A), f(0) \in H_{s+1/2}\}. \end{aligned} \tag{4.15}$$

PROOF. Let f be in the right hand side of (4.15). Then by Proposition 2.13 we choose $g \in \mathcal{H}_{s+1}(\mathbb{R}_+, A)$ with $g(0) = f(0)$ and put $f_1 := f - g$. Then $Df_1 \in \mathcal{H}_s(\mathbb{R}_+, A)$, $Pf_1(0) = 0$ and hence by the Regularity Theorem we have $f_1 \in \mathcal{H}_{s+1}(\mathbb{R}_+, A)$ and thus $f \in \mathcal{H}_{s+1}(\mathbb{R}_+, A)$. \square

This argument relies on the existence of at least one elliptic pair (P, P_+) . In Proposition 5.1 below we will see that the pair (P_+, P_+) indeed is elliptic.

Let $P \in \text{Op}^\mu(A)$ be an orthogonal projection such that D_P is self-adjoint. Then $\mathcal{D}(D_P^n) \subset \mathcal{H}_n(\mathbb{R}_+, A)$ already implies that P is n -regular. Namely, from complex interpolation we infer for $0 \leq k \leq n$

$$\begin{aligned} \mathcal{D}(D_P^k) &= [\mathcal{H}_0(\mathbb{R}_+, A), \mathcal{D}(D_P^n)]_{k/n} \\ &\subset [\mathcal{H}_0(\mathbb{R}_+, A), \mathcal{H}_n(\mathbb{R}_+, A)]_{k/n} \\ &= \mathcal{H}_k(\mathbb{R}_+, A). \end{aligned} \tag{4.16}$$

Corollary 4.6 asserts that D_P is self-adjoint if and only if P is regular and γ -symmetric. By Theorem 4.3 (2), $D_{P,\max} = D_P$ is also self-adjoint in this case. We now want to show that $D_{P,\max}$ may be self-adjoint also for non-regular γ -symmetric projections. We do not treat the description of self-adjoint extensions in full generality, we have singled out only the most tractable class of projections.

PROPOSITION 4.15. *Let $P \in \text{Op}^0(A)$ be a γ -symmetric orthogonal projection. If there is $C > 0$ such that for $\varepsilon \in (0, 1)$*

$$\|(I - P)(I + \varepsilon^2 A^2)^{-1}P\|_{H_{-1/2} \rightarrow H_{1/2}} \leq C, \quad (4.17)$$

then $D_{P,\max}$ is self-adjoint.

PROOF. In view of Theorem 4.3 (1), $D_{P,\max}$ is a closed operator with $D_{P,\max} \supseteq \overline{D_P} = D_{P,\max}^*$. Hence we need to show that $D_{P,\max}$ is symmetric. Let $f, g \in \mathcal{D}(D_{P,\max})$. Then using Lemma 2.15 we find

$$\begin{aligned} -(D_{P,\max}f, g) + (f, D_{P,\max}g) \\ = \lim_{\varepsilon \rightarrow 0} B_{-1/2}((I + \varepsilon^2 A^2)^{-1}\gamma(I - P)f(0), (I - P)g(0)) \\ = \lim_{\varepsilon \rightarrow 0} B_{-1/2}((I - P)(I + \varepsilon^2 A^2)^{-1}P\gamma f(0), g(0)). \end{aligned}$$

In H_0 the family $(I + \varepsilon^2 A^2)^{-1}$ converges to I strongly, as $\varepsilon \rightarrow 0$. Since $(I + \varepsilon^2 A^2)^{-1}$ commutes with $|A|$ we also have $\lim_{\varepsilon \rightarrow 0} (I + \varepsilon^2 A^2)^{-1} = I$ strongly in H_s , for each $s \in \mathbb{R}$. In particular, for $\xi \in H_{1/2}$ we have $\lim_{\varepsilon \rightarrow 0} (I - P)(I + \varepsilon^2 A^2)^{-1}P\xi = 0$ in $H_{1/2}$. Hence

$$(I - P)(I + \varepsilon^2 A^2)^{-1}P \in \mathcal{L}(H_{-1/2}, H_{1/2})$$

converges to 0 as $\varepsilon \rightarrow 0$, pointwise on a dense subset of $H_{-1/2}$. Consequently, the uniform norm bound implies the strong convergence, and $D_{P,\max}$ is symmetric. \square

We note some criteria for $(I - P)(I + \varepsilon^2 A^2)^{-1}P \in \mathcal{L}(H_{-1/2}, H_{1/2})$ to be bounded. First, boundedness is obvious if P and A^2 commute. More generally, we have

LEMMA 4.16. *If the commutator $[P, A^2]$ is in $\text{Op}^1(A)$, then (4.17) holds and hence $D_{P,\max}$ is self-adjoint.*

PROOF. Using the identity

$$(I - P)(I + \varepsilon^2 A^2)^{-1}P = \varepsilon^2(I - P)(I + \varepsilon^2 A^2)^{-1}[P, A^2](I + \varepsilon^2 A^2)^{-1},$$

we estimate

$$\begin{aligned} &\|(I - P)(I + \varepsilon^2 A^2)^{-1}P\|_{H_{-1/2} \rightarrow H_{1/2}} \\ &\leq \|I - P\|_{H_{1/2} \rightarrow H_{1/2}} \varepsilon^2 \| [P, A^2] (I + \varepsilon^2 A^2)^{-1} \|_{H_{-1/2} \rightarrow H_{1/2}} \\ &\leq \|I - P\|_{H_{1/2} \rightarrow H_{1/2}} \| [P, A^2] \|_{H_{3/2} \rightarrow H_{1/2}} \varepsilon^2 \| (I + \varepsilon^2 A^2)^{-1} \|_{H_{-1/2} \rightarrow H_{3/2}} \\ &\leq C. \end{aligned} \quad \square$$

If we restrict to $P \in \mathcal{P}_s(\Psi^0(A))$, with $\Psi^0(A)$ an algebra satisfying (3.31), then $[P, A^2] \in \text{Op}^1(A)$ is implied by the following condition prominent in Alain Connes' Noncommutative Differential Geometry:

$$(H, |A|, \Psi^0(A)) \text{ forms a spectral triple.} \quad (4.18)$$

Indeed, from $[|A|, B]$ bounded for $B \in \Psi^0(A)$, we deduce $[|A|, B] \in \text{Op}^0(A)$ as in [15, Lemma 1], wherefrom we easily derive $[P, A^2] \in \text{Op}^1(A)$. (4.18) will also be important in deriving the heat asymptotics in part IV of this work. This is plausible from the fact that for A a classical pseudodifferential operator with scalar principal symbol on a compact manifold, the algebra of classical pseudodifferential operators of order 0 satisfies (4.18).

We record the result.

PROPOSITION 4.17. *If $(H, |A|, \Psi^0(A))$ is a spectral triple, then $D_{P,\max}$ is self-adjoint for any $P \in \mathcal{P}_s(\Psi^0(A))$.*

Finally, we discuss the existence of non-regular $P \in \text{Op}^0(A)$.

PROPOSITION 4.18. *$D_{P_-, \max}$ is self-adjoint; but if A is unbounded, then P_- is not regular.*

PROOF. Since $[P_-, A^2] = 0$, the self-adjointness of $D_{P_-, \max}$ follows from Lemma 4.16.

Since A is unbounded and anticommutes with γ the operator $P_{\geq 1}(A)$ is unbounded, too. Hence we can find $u = P_{\geq 1}u \in H \setminus H_{1/2}$. Then the function

$$f(x) := e^{-Ax}u$$

is in $\mathcal{D}(D_{P_-, \max})$ but $f(0) \notin H_{1/2}$; in view of (4.6b), P_- cannot be regular. \square

More generally, we can prove:

PROPOSITION 4.19. *Let A be unbounded. If P is regular and $[P, A] \in \text{Op}^0(A)$, then $I - P$ is not regular. However, in this case $D_{I-P, \max}$ is self-adjoint.*

PROOF. Let $f \in \mathcal{D}(D^*)$. Since $[P, A] \in \text{Op}^0(A)$ one checks that $Pf, (I - P)f \in \mathcal{D}(D^*)$. Hence $Pf \in \mathcal{D}(D_{I-P, \max}), (I - P)f \in \mathcal{D}(D_{P, \max})$. If $I - P$ were regular we would get $\mathcal{D}(D^*) \subset \mathcal{H}_1(\mathbb{R}_+, A)$. In view of the Trace Theorem 2.12 this contradicts (4.4).

The self-adjointness of $D_{I-P, \max}$ follows from Lemma 4.16 since $[P, A^2] = [P, A]A + A[P, A] \in \text{Op}^1(A)$. \square

5. Criteria for regularity

We now study more closely the notion of n -regularity established in Definition 4.4.

PROPOSITION 5.1. *P_+ is n -regular for all $n \in \mathbb{Z}_+$ or, in other words, the pair (P_+, P_+) is elliptic.*

PROOF. For $n = 1$ this follows from Lemma 4.2.

Inductively, we assume that P_+ is n -regular. Let $f \in \mathcal{D}(D_{P_+}^{n+1})$, then $D_{P_+} f \in \mathcal{D}(D_{P_+}^n) \subset \mathcal{H}_n(\mathbb{R}_+, A)$ and consequently

$$(D_{P_+}^j f)(0) \in H_{n+1/2-j}, \quad 1 \leq j \leq n+1. \quad (5.1)$$

In view of Corollary 2.17 it remains to prove that $f(0) \in H_{n+1/2}$. Since $f \in \mathcal{D}(D_{P_+}^n) \subset \mathcal{H}_n(\mathbb{R}_+, A)$ we already have $f(0) \in H_{n-1/2}$. In view of Corollary 2.14 we may choose $h := e^{(n+1)}(0, (Df)(0), \dots, (D^n f)(0)) \in \mathcal{H}_{n+1}(\mathbb{R}, A)$ and put $f_1 := f - h$.

As in (4.5) we put $g(x) := \chi(x)e^{-Ax}f_1(0)$, $x \leq 0$. Then $g \in \mathcal{D}((D_-^*)^{n+1})$ and $(D_-^j g)(0) = (D_-^j f_1)(0)$, $0 \leq j \leq n$. Hence Proposition 2.16 implies $f_1 \in \mathcal{H}_{n+1}(\mathbb{R}_+, A)$ and thus $f \in \mathcal{H}_{n+1}(\mathbb{R}_+, A)$. \square

Now we are ready to state the analogue of Theorem 4.3 for n -regular projections:

PROPOSITION 5.2. *Let $P \in \text{Op}^0(A)$ be an orthogonal projection. The following statements are equivalent:*

- (i) P is n -regular.
- (ii) $r_+^{(k)}(\mathcal{D}(D_{P,\max}^{k+1})) \subset \bigoplus_{j=0}^k H_{k-j+1/2}$, $0 \leq k \leq n-1$.
- (iii) For $1 \leq k \leq n$ the following holds:
if $\xi \in H_{-1/2}$ and $P\xi = 0$, $P_-\xi \in H_{k-1/2}$, then $\xi \in H_{k-1/2}$. $\quad (5.2)$

PROOF. The equivalence of (i) and (ii) follows from Corollary 2.17.

(ii) \Rightarrow (iii): We proceed by induction on n . For $n = 1$ the assertion follows from Theorem 4.3.

Let P be n -regular. It remains to check the case $k = n$ in (5.2). Consider $\xi \in H_{-1/2}$, $P\xi = 0$, $P_-\xi \in H_{n-1/2}$. The induction hypothesis implies $\xi \in H_{n-3/2}$. In view of Corollary 2.14 choose $g := e^{(n-1)}(P_-\xi, 0, \dots, 0) \in \mathcal{H}_n(\mathbb{R}_+, A)$ and put

$$f(x) := \chi(x)e^{-Ax}P_+\xi + P_-g(x).$$

Then $f \in \mathcal{D}((D_P^*)^n)$ and hence by the n -regularity of P , $D_P^* = D_P$ and we have $f \in \mathcal{H}_n(\mathbb{R}_+, A)$, $\xi = f(0) \in H_{n-1/2}$.

(iii) \Rightarrow (i): Again we proceed by induction on n . For $n = 1$ the assertion follows from Theorem 4.3.

Assume (5.2) for $1 \leq k \leq n$. By the induction hypothesis P is $(n-1)$ -regular, so for $f \in \mathcal{D}(D_P^n)$ we have $Df \in \mathcal{D}(D_P^{n-1}) \subset \mathcal{H}_{n-1}(\mathbb{R}_+, A)$. Put $f_1 := P_-f$, then $Df_1 = P_+Df \in \mathcal{H}_{n-1}(\mathbb{R}_+, A)$, $P_+f_1(0) = 0$. In view of Proposition 5.1 and Proposition 4.8 we find $P_-f(0) = f_1(0) \in H_{n-1/2}$. Thus (5.2) implies $f(0) \in H_{n-1/2}$ and hence from Corollary 2.17 we infer $f \in \mathcal{H}_n(\mathbb{R}_+, A)$. \square

Next we clarify the relation between the notion ‘‘ellipticity’’ and ‘‘elliptic pair’’ (Definitions 4.9 and 4.10).

PROPOSITION 5.3. *Let $P \in \text{Op}^0(A)$ be a γ -symmetric orthogonal projection.*

- (1) *P is n -regular if and only if the operator $K := (I + A^2)^{1/4}TT^*(I + A^2)^{1/4}$, where $T = PP_+ + (I - P)P_-$ (cf. (3.5)), is regular at $0, 1, \dots, n - 1$ in the sense of Definition 4.10. In particular, the pair (P, P_+) is elliptic if and only if K is elliptic.*
- (2) *The pair (P, P_+) is elliptic if and only if for all $s \in \mathbb{R}$ the following holds:
If $\xi \in H_{-\infty}$ and $P\xi = 0, P_-\xi \in H_s$, then $\xi \in H_s$. (5.3)*

PROOF. We remark first that (5.2) and (5.3) are, in fact, symmetric in P and P_- . Namely, (5.3) is clearly a consequence of

$$\xi \in H_{-\infty}, P\xi \in H_t, \text{ and } P_-\xi \in H_s \text{ imply } \xi \in H_{\min(s,t)}. \quad (5.3')$$

But applying (5.3) to $\eta := \xi - P\xi$ shows that (5.3') also follows (5.3), so both statements are equivalent; a similar reasoning works for (5.2).

By the γ -symmetry of P and P_+ , (5.2) resp. (5.3) also hold with $I - P$ and P_+ in place of P and P_- .

With these preparations we prove (1): Let K be regular at $0, \dots, n - 1$. In view of Proposition 5.2 (iii), we consider $\xi \in H_{-1/2}$ with $P\xi = 0$ and $P_-\xi \in H_{k-1/2}$ for some $1 \leq k \leq n$. We put $\eta := (I + A^2)^{-1/4}\xi \in H_0$ and find

$$K\eta = (I + A^2)^{1/4}(I - P)P_-\xi \in H_{k-1}.$$

Since K is regular at $k - 1$ we conclude $\eta \in H_k$ and thus $\xi \in H_{k-1/2}$.

Conversely, let P be n -regular and consider $\xi \in H_0$ with $K\xi \in H_k$ for some $0 \leq k \leq n - 1$. $K\xi \in H_k$ implies in view of Remark 4.12

$$PP_+P\eta, (I - P)P_-(I - P)\eta \in H_{k+1/2}, \quad \eta := (I + A^2)^{1/4}\xi.$$

We invoke the n -regularity of P and infer from

$$P(P_+P\eta) \in H_{k+1/2}, \quad P_-(P_+P\eta) = 0$$

that $P_+P\eta \in H_{k+1/2}$. Proceeding in this way we arrive at $P\eta \in H_{k+1/2}$. Analogously one derives $(I - P)\eta \in H_{k+1/2}$, hence $\eta \in H_{k+1/2}$ and finally $\xi \in H_{k+1}$. Hence K is n -regular.

Thus the first assertion of (1) is proved. The second assertion of (1) as well as (2) follow from the first one and Proposition 4.11. \square

From now on we will use the axioms (3.31) on the algebra $\Psi^0(A)$.

THEOREM 5.4. *Let $P \in \Psi^0(A)$ be a γ -symmetric orthogonal projection. If the pair (P, P_+) is Fredholm, then it is elliptic.*

PROOF. Assume first that (P, P_+) is an invertible pair. Then

$$T = PP_+ + (I - P)P_- \in \Psi^0(A)$$

is invertible (by Remark 3.5 and Corollary 3.4). By axiom (3.31b) we then have $T^{-1} \in \Psi^0(A)$. Now let $\xi \in H_{-\infty}$, $P_- \xi = 0$, $P \xi \in H_s$. Then

$$\xi = T^{-1}T\xi = T^{-1}PP_+\xi = T^{-1}P\xi \in H_s. \quad (5.4)$$

If $P \in \mathcal{P}(\Psi^0(A))$ is arbitrary, then we write $P = P' + P''$ as in (3.12). The proof of Theorem 3.12 shows that $P' + P''_+ \in \mathcal{P}_s(\Psi^0(A))$; by (3.35) the pair $(P' + P''_+, P_+)$ is invertible. By the first part of this proof, $(P' + P''_+, P_+)$ also is an elliptic pair. By Lemma 2.4 the finite rank operators P'' and P''_+ are smoothing, hence $(P' + P''_+)\xi = P\xi + (P''_+ - P'')\xi \in H_s$ and as before we see that $\xi \in H_s$. \square

If A is a discrete operator, one can get a better result. First we state the abstract elliptic regularity theorem for scales of Hilbert spaces:

PROPOSITION 5.5. *Let $(H_s)_{s \in \mathbb{R}}$ be a scale of Hilbert spaces such that for $s' > s$ the embedding $H'_s \hookrightarrow H_s$ is compact. Let $T \in \text{Op}^\mu := \text{Op}^\mu((H_s)_{s \in \mathbb{R}})$, $\mu > 0$. Assume that T is regular at 0. Then*

- (1) *For $0 \leq s \leq \mu$, T extends to a Fredholm operator $H_s \rightarrow H_{s-\mu}$ with index independent of s .*
- (2) *Let S be the generalized inverse of T defined by $ST\xi = \xi$ for $\xi \in \ker T^\perp$, and $S\xi := 0$ for $\xi \in \text{im } T^\perp$, where \perp is taken in H_0 . Then S extends by continuity to a bounded linear operator $H_s \rightarrow H_{s+\mu}$, $-\mu \leq s \leq 0$.*

If, in addition, T is elliptic then S is a parametrix in the sense that

$$I - TS, I - ST \in \text{Op}^{-\infty},$$

and for all $s \in \mathbb{R}$, T extends to a Fredholm operator $H_s \rightarrow H_{s-\mu}$.

PROOF. We first consider T as an unbounded operator in H_0 ; then T is a closed operator with domain H_μ . To see this let $(x_n)_{n \in \mathbb{N}} \subset H_\mu$ be a sequence such that $x_n \rightarrow x$, $Tx_n \rightarrow \xi$ in H_0 . Since $T \in \text{Op}^\mu$ we have the equality $Tx = \xi$ in $H_{-\mu}$, and the regularity of T at 0 implies $x \in H_\mu$.

By the same argument, T^t induces a closed operator with domain H_μ , which is the adjoint, T^* , of $T : H_\mu \rightarrow H_0$.

By assumption, $H_\mu \hookrightarrow H_0$ is compact. Since the domains of T and T^* are both compactly embedded, T and T^* are Fredholm operators $H_\mu \rightarrow H_0$. By duality, T and T^t induce Fredholm operators $H_0 \rightarrow H_{-\mu}$ hence, by complex interpolation, from $H_s \rightarrow H_{s-\mu}$, $0 \leq s \leq \mu$.

By definition, the generalized inverse S maps $H_0 \rightarrow H_\mu$ and its adjoint, S^* , is a generalized inverse of T^* . By duality and complex interpolation, again, S and S^* induce continuous maps $S, S^t : H_s \rightarrow H_{s+\mu}$, $-\mu \leq s \leq 0$.

The operators $I - ST, I - TS$ are orthogonal projections in H_0 with $(I - ST)(H_0) = \ker T \subset H_\mu$, $(I - TS)(H_0) = \ker T^t \subset H_\mu$. Since $I - TS, I - ST$ are orthogonal projections, by duality, they map $H_{-\mu} \rightarrow H_0$ and hence $H_{-\mu} \rightarrow H_\mu$. This proves that $\ker T \restriction H_s$ is independent of s for $0 \leq s \leq \mu$.

If T is elliptic then the finite rank operators $I - TS$ and $I - ST$ map $H_0 \rightarrow H_\infty$ and Lemma 2.4 implies $I - TS, I - ST \in \text{Op}^{-\infty}$. \square

Now we can state the main result of this section:

THEOREM 5.6. *Let A be discrete. For a γ -symmetric orthogonal projection $P \in \Psi^0(A)$ the following statements are equivalent:*

- (i) P is regular.
- (ii) (P, P_+) is an elliptic pair.
- (iii) (P, P_+) is a Fredholm pair.

PROOF. (i) \Rightarrow (iii): Let P be a regular projection. By Proposition 5.3, this is equivalent to the fact that $K := (I + A^2)^{1/4}TT^*(I + A^2)^{1/4}$, with $T = PP_+ + (I - P)P_-$, is regular at 0. From Proposition 5.5 we infer that K is Fredholm $H_s(A) \rightarrow H_{s-1}(A)$, $0 \leq s \leq 1$. Hence TT^* is Fredholm $H_s \rightarrow H_s$, $-\frac{1}{2} \leq s \leq \frac{1}{2}$, in particular, (P, P_+) is a Fredholm pair.

(iii) \Rightarrow (ii): This follows from Theorem 5.4.

(ii) \Rightarrow (i): This follows from Theorem 4.3 and the definition of ellipticity. \square

We note that the implications ”(i) \Rightarrow (iii)” and ”(ii) \Rightarrow (i)” remain valid if we assume only that P is a γ -symmetric orthogonal projection in $\text{Op}^0(A)$.

EXAMPLE 5.7. In [12, Sec. 3] we described a special class of orthogonal projections defining generalized Atiyah–Patodi–Singer boundary value problems. We now discuss these projections in some detail:

Let P be a γ -symmetric orthogonal projection. Assume that

$$[P, |A|] = 0, \tag{5.5}$$

$$PAP = \alpha|A|P \text{ for some } \alpha > -1. \tag{5.6}$$

(5.5) implies that $P \in \text{Op}^0(A)$.

PROPOSITION 5.8. *Let P be a γ -symmetric orthogonal projection satisfying (5.5) and (5.6). Then the following assertions hold:*

- (1) *The pair (P, P_+) is elliptic.*
- (2) *If $\dim \ker A < \infty$ then (P, P_+) is a Fredholm pair. If $\ker A = 0$ then (P, P_+) is an invertible pair.*

PROOF. For $\lambda > 0$ consider the operator

$$P_\lambda := \frac{1}{2}(|A| + \lambda)^{-1}(A + |A|). \tag{5.7}$$

P_λ converges to $P_{>0}(A)$ strongly, as $\lambda \rightarrow 0+$. In view of (5.5), (5.6) we have

$$\begin{aligned} PP_\lambda P &= (|A| + \lambda)^{-1}|A|\frac{1+\alpha}{2}P \\ &\rightarrow (P_{<0}(A) + P_{>0}(A))\frac{1+\alpha}{2}P \end{aligned} \tag{5.8}$$

strongly, as $\lambda \rightarrow 0+$. Hence

$$PP_{>0}(A)P = (P_{<0}(A) + P_{>0}(A))\frac{1+\alpha}{2}P, \quad (5.9)$$

and consequently we infer that

$$PP_+P = \frac{1+\alpha}{2}P + R, \quad (5.10)$$

where

$$R = P(P_+ - P_{>0}(A))P - \frac{1+\alpha}{2}P_0P \in \text{Op}^{-\infty}(A). \quad (5.11)$$

By construction, if $\dim \ker A < \infty$, then R is of finite rank and if $\ker A = 0$ then $R = 0$. For $T := PP_+ + (I - P)P_-$ we find

$$TT^* = \frac{1+\alpha}{2}I + R + \gamma R\gamma^*. \quad (5.12)$$

Since R is smoothing, TT^* and thus the pair (P, P_+) is elliptic, in view of Proposition 5.3. If $\dim \ker A < \infty$ then TT^* and thus (P, P_+) is Fredholm. Finally, if $\ker A = 0$ then TT^* and hence (P, P_+) is invertible. \square

PROPOSITION 5.9. *Let $P \in \text{Op}^0(A)$ be a γ -symmetric orthogonal projection.*

- (1) *If $(I - P)P_+(I - P) \in \text{Op}^{-\varepsilon}(A)$ for some $\varepsilon > 0$, then the pair (P, P_+) is elliptic.*
- (2) *Let $P_1 \in \text{Op}^0(A)$ be another γ -symmetric orthogonal projection. If (P, P_+) is elliptic and $(P - P_1) \in \text{Op}^{-\varepsilon}(A)$ for some $\varepsilon > 0$, then (P_1, P_+) is also elliptic.*

PROOF. (1) Let $x \in H_{s_0}$, for some $s_0 \in \mathbb{R}$, $Px = 0$, $P_-x \in H_s$. We have

$$0 = Px = PP_+x + PP_-x,$$

thus $PP_+x = -PP_-x \in H_s$. This implies

$$\begin{aligned} P_+x &= PP_+x + (I - P)P_+(I - P)x \\ &= -PP_-x + (I - P)P_+(I - P)x \\ &\in H_{\min(s, s_0 + \varepsilon)}. \end{aligned}$$

Iterating this procedure we conclude $x \in H_s$.

- (2) Let $x \in H_{s_0}$, $P_1x = 0$, $P_-x \in H_s$. Then

$$Px = (P - P_1)x \in H_{s_0 + \varepsilon},$$

hence $x \in H_{\min(s, s_0 + \varepsilon)}$. Again, we reach the conclusion by iterating this argument. \square

Now we can present the

PROOF OF THEOREM 1.3. In this proof D_P denotes the operator defined in (4.1), i.e. $\mathcal{D}(D_P) = \{u \in \mathcal{H}_1(\mathbb{R}_+, A) \mid Pu(0) = 0\}$, and we put $D_{P,0} := D_P \upharpoonright_{\mathcal{D}_P} := \{f \in C_0^\infty(\mathbb{R}_+, H_1) \mid Pf(0) = 0\}$. Note that the D_P in the formulation of Theorem 1.3 is the $D_{P,0}$ in the present notation.

By Corollary 4.7 \mathcal{D}_P is a core for D_P and hence D_P is the closure of $D_{P,0}$. Furthermore, in view of (1.13) and Theorem 4.3 (1) we have $D_P^* = D_{P,\max}$. From (1.23) and Theorem 5.4 we infer that P is a regular projection and hence in view of the three equivalent characterizations of regularity in Theorem 4.3 (2) we have $D_P = D_{P,\max} = D_P^*$. This proves the first part of Theorem 1.3.

To prove the second part we assume that A is discrete and that D_P is self-adjoint on $\{f \in \mathcal{H}_1(\mathbb{R}_+, A) \mid Pf(0) = 0\}$. Hence P is regular by Theorem 4.3. Then (1.23) is a consequence of Theorem 5.6. (1.13) follows from Corollary 4.6. \square

6. Variable coefficients and second order operators

We now study the model operator (1.10) with variable coefficients. In most applications we will need the following results only in a small neighborhood of $x = 0$. Therefore, we may assume that the operator has constant coefficients at infinity. More precisely, we consider the differential operator

$$\begin{aligned} D &= \gamma\left(\frac{d}{dx} + A(x)\right) \\ &=: \gamma\left(\frac{d}{dx} + A_0\right) + x\gamma A_1(x) \\ &=: D_0 + x\gamma A_1(x), \end{aligned} \tag{6.1}$$

where (1.9) now holds with $A(x)$ in place of A , for all x , and we assume in addition that

$A(x) \in \text{Op}^1(A_0)$ is self-adjoint with domain $H_1(A_0)$ and elliptic (6.2a) with respect to the scale $(H_s(A_0))_{s \in \mathbb{R}}$,

for all $s \in \mathbb{R}$, the map

$$\mathbb{R} \ni x \mapsto (I + A_0^2)^s A(x)(I + A_0^2)^{-1/2-s} \in \mathcal{L}(H_0(A_0)) \tag{6.2b}$$

is smooth,

$$A_1(x) = 0 \text{ for } |x| \geq R > 0. \tag{6.2c}$$

Note that, from (1.9)

$$\gamma A_1(x) + A_1(x)\gamma = 0, \quad \text{for all } x. \tag{6.2d}$$

(6.2a) implies that

$$H_s(A(x)) = H_s(A_0) \quad \text{for } x, s \in \mathbb{R}, \tag{6.3}$$

and (6.2b) implies

$$A^{(j)}(x) \in \text{Op}^1(A_0), \quad \text{for } j \in \mathbb{Z}_+. \quad (6.4)$$

We abbreviate $H_s := H_s(A_0)$. As in the constant coefficient case we are interested in D as an unbounded operator in $L^2(\mathbb{R}_+, H)$ with domain $C_0^\infty((0, \infty), H_\infty)$; the corresponding operator in $L^2(\mathbb{R}, H)$ with domain $C_0^\infty(\mathbb{R}, H_\infty)$ will be denoted by \tilde{D} . Then D, \tilde{D} are symmetric operators in the respective Hilbert spaces. We have

$$D^2 = -\frac{d^2}{dx^2} + A(x)^2 - A'(x). \quad (6.5)$$

Our analysis of the constant coefficient case applies to D_0 in (6.1). In particular, \tilde{D}_0 is essentially self-adjoint on $C_0^\infty(\mathbb{R}, H_\infty) \subset L^2(\mathbb{R}, H)$. Its closure has domain $\mathcal{H}_1(\mathbb{R}, A_0)$ and will also be denoted by \tilde{D}_0 . Moreover, $\mathcal{H}_1(\mathbb{R}, A_0) \subset \mathcal{D}(\tilde{D})$.

We first state the analogue of Lemma 2.15.

LEMMA 6.1. (1) $\mathcal{D}(D^*) \subset \{f \in L^2(\mathbb{R}_+, H) \mid f' \in L^2(\mathbb{R}_+, H_{-1})\}$ and we have a continuous restriction map $r : \mathcal{D}(D^*) \rightarrow H_{-1/2}, f \mapsto f(0)$.

(2) For $f, g \in \mathcal{D}(D^*)$ we have

$$-(D^*f, g) + (f, D^*g) = \lim_{\varepsilon \rightarrow 0} \left(\gamma(\pm \varepsilon A_0 + i)^{-1} f(0), (\varepsilon A_0 + i)^{-1} g(0) \right).$$

If $f(0)$ or $g(0)$ lies in $H_{1/2}$ then

$$-(D^*f, g) + (f, D^*g) = B_{\mp 1/2}(\gamma f(0), g(0)). \quad (6.6)$$

PROOF. The proof is almost identical to the proof of Lemma 2.15. We only have to note that for $f \in \mathcal{D}(D^*)$ the family

$$f_\varepsilon(x) := i(\varepsilon A(x) + i)^{-1} f(x)$$

satisfies the relations $f_\varepsilon \in L^2(\mathbb{R}_+, H)$, $\lim_{\varepsilon \rightarrow 0} f_\varepsilon = f$,

$$f'_\varepsilon(x) = -\varepsilon(\varepsilon A(x) + i)^{-1} A'(x) f_\varepsilon + i(\varepsilon A(x) + i)^{-1} f'(x) \in L^2(\mathbb{R}_+, H),$$

and D^*f_ε has uniformly bounded norm. Thus $D^*f_\varepsilon \rightharpoonup D^*f$ as shown by the next lemma. \square

The last proof used the following simple but useful lemma, which allows to describe a core of an unbounded operator in terms of weak convergence.

LEMMA 6.2. Let D be a closed operator in a Hilbert space \mathcal{H} .

- (1) Let $f \in \mathcal{H}$ and $(f_n) \subset \mathcal{D}(D)$ be a sequence such that (f_n) converges weakly to $f \in \mathcal{H}$ and (Df_n) has uniformly bounded norm in \mathcal{H} . Then $f \in \mathcal{D}(D)$ and $Df_n \rightharpoonup Df$.
- (2) Let $\mathcal{E} \subset \mathcal{D}(D)$ be a linear subspace such that for every $f \in \mathcal{D}(D)$ there is a sequence $(f_n) \subset \mathcal{E}$ with $f_n \rightharpoonup f$ and (Df_n) bounded. Then \mathcal{E} is a core for D .

PROOF. (1) For every $g \in \mathcal{D}(D^*)$ we have

$$(Df_n, g) = (f_n, D^*g) \xrightarrow{n \rightarrow \infty} (f, D^*g), \quad (6.7)$$

i.e. the bounded sequence (Df_n) converges weakly on a dense subspace and hence is weakly convergent. Let h be the weak limit of (Df_n) . Then in view of (6.7) we have $(h, g) = (f, D^*g)$ for all $g \in \mathcal{D}(D^*)$, thus $f \in \mathcal{D}(D)$ and $Df = h$.

(2) To prove that \mathcal{E} is a core for D we have to show that if $g \in \mathcal{D}(D)$ with $0 = (g, f) + (Dg, Df)$ for all $f \in \mathcal{E}$ then $g = 0$. Given such a g we choose $(f_n) \subset \mathcal{E}$ with $f_n \rightharpoonup g$ and $Df_n \rightharpoonup Dg$, using (1). Then

$$(g, g) + (Dg, Dg) = \lim_{n \rightarrow \infty} \{(g, f_n) + (Dg, Df_n)\} = 0. \quad \square$$

As in the constant coefficient case we want to find boundary conditions defining self-adjoint extensions of D . Our main tool will be (a variant of) the Kato–Rellich Theorem so we need to estimate relative bounds.

LEMMA 6.3. *Let $B(x), x \in \mathbb{R}$, be a family of operators of order 1 satisfying (6.2b). Then for $\varepsilon > 0$ and $n \in \mathbb{Z}_+$ there exists $C(\varepsilon, n, B)$ such that for $f \in \mathcal{H}_{n+1}(\mathbb{R}, A_0)$ we have the estimate*

$$\begin{aligned} \|Bf\|_{\mathcal{H}_n} &\leq c_n \left(\sup_{x \in \mathbb{R}} \max \left(\|B(x)T^{-1}\|_{\mathcal{L}(H_0)}, \|T^n B(x)T^{-1-n}\|_{\mathcal{L}(H_0)} \right) + \varepsilon \right) \|f\|_{\mathcal{H}_{n+1}} \\ &\quad + C(\varepsilon, n, B) \|f\|_{\mathcal{H}_0}. \end{aligned}$$

Here, c_n is a universal constant depending only on n and $T := (I + A_0^2)^{1/2}$.

PROOF. In this proof, c_n and $C(\cdot)$ denote generic constants depending on their respective arguments.

For $f \in \mathcal{H}_1(\mathbb{R}, A_0)$ we have

$$\begin{aligned} \|Bf\|_{\mathcal{H}_0}^2 &= \int_{\mathbb{R}} \|B(x)f(x)\|_{H_0}^2 dx \\ &\leq \sup_{x \in \mathbb{R}} \|B(x)T^{-1}\|_{\mathcal{L}(H_0)}^2 \int_{\mathbb{R}} \|Tf(x)\|_{H_0}^2 dx \\ &= \sup_{x \in \mathbb{R}} \|B(x)T^{-1}\|_{\mathcal{L}(H_0)}^2 \|Tf\|_{\mathcal{H}_0(\mathbb{R}, A_0)}^2. \end{aligned} \quad (6.8)$$

Using this estimate and Proposition 2.10 we find

$$\begin{aligned}
& \|Bf\|_{\mathcal{H}_n} \\
& \leq c_n \sum_{j=0}^n \left\| \left(\frac{d}{dx} \right)^j T^{n-j} B f \right\|_{\mathcal{H}_0} \\
& \leq c_n \sum_{j=0}^n \sum_{i=0}^j \left\| T^{n-j} B^{(i)} f^{(j-i)} \right\|_{\mathcal{H}_0} \\
& \leq c_n \sum_{j=0}^n \sum_{i=0}^j \sup_{x \in \mathbb{R}} \left\| T^{n-j} B^{(i)}(x) T^{j-n-1} \right\|_{\mathcal{L}(H_0)} \left\| T^{n+1-j} f^{(j-i)} \right\|_{\mathcal{H}_0},
\end{aligned}$$

where in the last inequality we have used (6.8) with $T^{n-j} B^{(i)} T^{j-n}$ in place of B and $T^{n-j} f^{(j-i)}$ in place of f . We treat the summands with $i = 0$ and $i \neq 0$ separately. Summands with $i = 0$ are estimated using the following inequality which follows from complex interpolation:

$$\begin{aligned}
& \|T^{n-j} B(x) T^{j-n-1}\|_{\mathcal{L}(H_0)} \\
& \leq \max(\|B(x) T^{-1}\|_{\mathcal{L}(H_0)}, \|T^n B(x) T^{-n-1}\|_{\mathcal{L}(H_0)}). \quad (6.9a)
\end{aligned}$$

For $i > 0$ we estimate in view of Proposition 2.10 and (2.13)

$$\begin{aligned}
& \|T^{n+1-j} f^{(j-i)}\|_{\mathcal{H}_0} \leq c_n \|f^{(j-i)}\|_{\mathcal{H}_{n+1-j}} \\
& \leq c_n \|f\|_{\mathcal{H}_{n+1-i}} \\
& \leq \varepsilon \|f\|_{\mathcal{H}_{n+1}} + C(\varepsilon, n) \|f\|_{\mathcal{H}_0}. \quad (6.9b)
\end{aligned}$$

The last inequality follows from $i > 0$, the fact that $\mathcal{H}_s(\mathbb{R}, A) = H_s(\tilde{D})$ (2.11), and the Spectral Theorem. The lemma is proved. \square

Next we note a variant of the Kato–Rellich Theorem.

PROPOSITION 6.4. *Let S be a self-adjoint operator in the Hilbert space H and let $R \in \text{Op}^1(S)$ be a symmetric operator. Assume that for fixed $N \in \mathbb{Z}_+$ and $\xi \in H_\infty(S)$ we have the estimates*

$$\|R\xi\|_{H_0(S)} \leq b\|S\xi\|_{H_0(S)} + c\|\xi\|_{H_0(S)}, \quad (6.10a)$$

$$\|R\xi\|_{H_{N-1}(S)} \leq b\|S\xi\|_{H_{N-1}(S)} + c\|\xi\|_{H_0(S)}, \quad (6.10b)$$

with $b < 1$ and $c > 0$.

Then the operator $S + R$ is self-adjoint with domain $H_1(S)$ and regular at $0 \leq k \leq N - 1$.

PROOF. The estimates (6.10) show that for $0 < \varepsilon < 1 - b$ there is a $\lambda_0 > 0$ such that for $\lambda \geq \lambda_0$

$$\|R(S - i\lambda)^{-1}\|_{\mathcal{L}(H_s(S))} \leq b + \varepsilon < 1. \quad (6.11)$$

A priori, (6.11) holds for $s = 0$ and $s = N - 1$, but by complex interpolation it holds for $0 \leq s \leq N - 1$. Thus the resolvent

$$(S + R - i\lambda)^{-1} = (S - i\lambda)^{-1} \sum_{n=0}^{\infty} (-1)^n (R(S - i\lambda)^{-1})^n \quad (6.12)$$

converges in $\mathcal{L}(H_s(S), H_{s+1}(S))$, $0 \leq s \leq N - 1$. As in the proof of the implication "i) \Rightarrow ii)" of Proposition 4.11 we now conclude that $S + R$ is regular at $0 \leq s \leq N - 1$. Of course, the self-adjointness of $S + R$ with domain $H_1(S)$ also follows from (6.12) (as in the proof of the Kato–Rellich Theorem). \square

Now we can prove the main result of this section, the generalization of the Regularity Theorem 4.13 to variable coefficients.

THEOREM 6.5 (Regularity Theorem). *Assume (6.1)–(6.2).*

- (1) *The operator \tilde{D} is elliptic with respect to the scale of Hilbert spaces $(\mathcal{H}_s(\mathbb{R}, A_0))_{s \in \mathbb{R}}$. In particular, \tilde{D} is essentially self-adjoint and $\mathcal{D}(\tilde{D}) = \mathcal{H}_1(\mathbb{R}, A_0)$.*
- (2) *Let $P \in \text{Op}^0(A)$ be a γ -symmetric orthogonal projection.*
 - (i) *The pair (P, P_+) is elliptic if and only if for all $s \in \mathbb{R}_+$ the relations*

$$\begin{aligned} D^* f = g &\in \mathcal{H}_s(\mathbb{R}_+, A), \quad f \in L^2(\mathbb{R}_+, H), \\ Pf(0) &= 0, \end{aligned} \quad (6.13)$$

imply $f \in \mathcal{H}_{s+1}(\mathbb{R}_+, A)$.

In other words, in this case the operator D_P defined by

$$D_P := D^* \upharpoonright \mathcal{D}(D_{0,P}) = \{f \in \mathcal{H}_1(\mathbb{R}_+, A_0) \mid Pf(0) = 0\}$$

fulfills the equivalent conditions (i)–(iii) of Proposition 4.11'. In particular, D_P is self-adjoint.

- (ii) *P is regular if and only if the operator D_P defined in (i) is self-adjoint.*

PROOF. (1) By Proposition 4.11 and Remark 4.12 2., it suffices to prove the regularity at all $n \in \mathbb{Z}_+$. Fix $x_0 \in \mathbb{R}$ and write

$$A(x) = A(x_0) + (x - x_0)A_1(x_0, x).$$

From (6.2b) we infer $A_1(x_0, x) \in \text{Op}^1(A_0)$ and in view of (6.2a) we have $H_s(A(x_0)) = H_s(A_0)$ and $\text{Op}^\mu(A(x_0)) = \text{Op}^\mu(A_0)$ for all $s, \mu \in \mathbb{R}$.

In view of Lemma 6.3 we may choose $\varphi, \psi \in C_0^\infty(\mathbb{R})$ with $\varphi \equiv 1$ in a neighborhood of x_0 and $\psi \equiv 1$ in a neighborhood of $\text{supp } \varphi$ such that for the operator

$$B := (x - x_0)\psi(x)\gamma A_1(x_0, x)$$

we have, for a fixed n ,

$$\begin{aligned} \|Bf\|_{\mathcal{H}_n} &\leq \tilde{b}\|f\|_{\mathcal{H}_{n+1}} + C(n)\|f\|_0 \\ &\leq \tilde{b}c_n\|\gamma(\frac{d}{dx} + A(x_0))f\|_{\mathcal{H}_n} + C'(n)\|f\|_0, \end{aligned} \quad (6.14)$$

and

$$\|Bf\|_0 \leq \tilde{b}\|f\|_{\mathcal{H}_1} + C(0)\|f\|_0 \leq \tilde{b}c_0\|\gamma(\frac{d}{dx} + A(x_0))f\|_0 + C'(0)\|f\|_0, \quad (6.15)$$

with \tilde{b} so small that $b := \tilde{b} \max(c_0, c_n) < 1$. Hence $B(x)$ is $\gamma(\frac{d}{dx} + A(x_0))$ -bounded with relative bound $b < 1$ for both the \mathcal{H}_0 and the \mathcal{H}_n -norm.

Now consider $f \in \mathcal{H}_0(\mathbb{R}, A_0)$ with $\tilde{D}f = g \in \mathcal{H}_n(\mathbb{R}, A_0)$. By Lemma 2.8 and Proposition 6.4 the operator

$$\tilde{D}(x_0) := \gamma(\frac{d}{dx} + A(x_0) + (x - x_0)\psi(x)A_1(x_0, x)) \quad (6.16)$$

is self-adjoint with domain $H_1(A_0)$ and regular at all $0 \leq s \leq n$.

Assume that we already know that $f \in \mathcal{H}_t(\mathbb{R}, A_0)$. Then

$$\tilde{D}(x_0)^*(\varphi f) = \tilde{D}^*(\varphi f) = \gamma\varphi'f + \varphi\tilde{D}^*f \in \mathcal{H}_{\min(n,t)}, \quad (6.17)$$

and consequently $\varphi f \in \mathcal{H}_{\min(n,t)+1}(\mathbb{R}, A_0)$.

Since x_0 was arbitrary we have proved $f \in \mathcal{H}_{\min(n,t)+1,\text{loc}}(\mathbb{R}, A_0)$.

To prove that $f \in \mathcal{H}_{\min(n,t)+1}(\mathbb{R}, A_0)$ we choose a cut-off function $\varphi \in C_0^\infty(\mathbb{R})$ with $\varphi \upharpoonright [-R, R] \equiv 1$. Then $\varphi f \in \mathcal{H}_{\min(n,t)+1}(\mathbb{R}, A_0)$ and in view of (6.2c) we have $(1 - \varphi)f \in \mathcal{D}(\tilde{D}_0^{n+1}) = \mathcal{H}_{n+1}(\mathbb{R}, A_0)$. (1) is proved.

(2i) We assume that (P, P_+) is elliptic and fix an integer $n \geq 0$. By the Regularity Theorem 4.13, the operator $D_{0,P}$, with D_0 from (6.1), induces a closed operator in $\mathcal{H}_n(\mathbb{R}_+, A_0)$ with domain $\mathcal{D}(D_{0,P}) \cap \mathcal{H}_{n+1}(\mathbb{R}_+, A_0)$. Hence, for $f \in \mathcal{D}(D_{0,P}) \cap \mathcal{H}_{n+1}(\mathbb{R}_+, A_0)$ there is an estimate

$$\begin{aligned} \|f\|_{\mathcal{H}_{n+1}(\mathbb{R}_+, A_0)} &\leq c(\|D_{0,P}f\|_{\mathcal{H}_n(\mathbb{R}_+, A_0)} + \|f\|_{\mathcal{H}_n(\mathbb{R}_+, A_0)}) \\ &\leq c\|D_{0,P}f\|_{\mathcal{H}_n(\mathbb{R}_+, A_0)} + \frac{1}{2}\|f\|_{\mathcal{H}_{n+1}(\mathbb{R}_+, A_0)} + c_{1/2}\|f\|_0, \end{aligned} \quad (6.18)$$

thus

$$\|f\|_{\mathcal{H}_{n+1}(\mathbb{R}_+, A_0)} \leq c(\|D_{0,P}f\|_{\mathcal{H}_n(\mathbb{R}_+, A_0)} + \|f\|_0). \quad (6.19)$$

In view of Lemma 6.3 we can thus choose cut-off functions φ, ψ near 0 as in the first part of this proof (cf. (6.14), (6.15)) such that $x\psi(x)\gamma A_1(x)$ is $D_{0,P}$ -bounded with relative bound $b < 1$, simultaneously for the $\mathcal{H}_0(\mathbb{R}_+, A_0)$ and the $\mathcal{H}_n(\mathbb{R}_+, A_0)$ -norm.

Proposition 6.4 does not apply directly with $R = x\psi(x)\gamma A_1(x)$ and $S = D_{0,P}$ since we do not necessarily have $R \in \text{Op}^1(D_{0,P})$. However, an inspection of the proof of Proposition 6.4 shows that

$$\tilde{D}_{0,P} := D_{0,P} + x\gamma\psi(x)A_1(x)$$

is self-adjoint with domain $\mathcal{H}_1(\mathbb{R}_+, A_0)$ and for $0 \leq t \leq n$ the following holds (cf. Proposition 4.11' versus Proposition 4.11):

$$f \in \mathcal{D}(\tilde{D}_{0,P}^*), \quad \tilde{D}_{0,P}^* f \in \mathcal{H}_t(\mathbb{R}_+, A_0) \implies f \in \mathcal{H}_{t+1}(\mathbb{R}_+, A_0).$$

Now consider f satisfying (6.13). Assume we already know $f \in \mathcal{H}_t(\mathbb{R}_+, A_0)$. As in (6.17) we conclude $\varphi f \in \mathcal{H}_{\min(n,t)+1}(\mathbb{R}_+, A_0)$. Using part (1) of the theorem we infer from

$$\tilde{D}^*(1 - \varphi)f = -\gamma\varphi'f + (1 - \varphi)D^*f \in \mathcal{H}_{\min(n,t)}(\mathbb{R}, A_0)$$

that also $(1 - \varphi)f \in \mathcal{H}_{\min(n,t)+1}(\mathbb{R}_+, A_0)$.

Conversely, assume that (6.13) implies $f \in \mathcal{H}_{s+1}(\mathbb{R}_+, A_0)$. Then we reverse the roles of D_P and $D_{0,P}$; i.e. (6.13) implies that D_P induces a closed operator in $\mathcal{H}_n(\mathbb{R}_+, A_0)$ with domain $\mathcal{D}(D_{0,P}) \cap \mathcal{H}_{n+1}(\mathbb{R}_+, A_0)$. Hence, the estimates (6.18) and (6.19) hold with D_P in place of $D_{0,P}$. Then we choose cut-off functions φ, ψ as before such that $x\gamma\psi(x)A_1(x)$ is D_P -bounded with relative bound $b < 1$, simultaneously for the $\mathcal{H}_0(\mathbb{R}_+, A_0)$ and the $\mathcal{H}_n(\mathbb{R}_+, A_0)$ -norm; as before $n \geq 0$ is some fixed integer.

Then we see again that the operator

$$D_{P,\psi} := D_P - x\gamma\psi(x)A_1(x) = D_{0,P} + x(1 - \psi(x))\gamma A_1(x)$$

satisfies

$$f \in \mathcal{D}(\tilde{D}_{P,\psi}^*), \quad \tilde{D}_{P,\psi}^* f \in \mathcal{H}_t(\mathbb{R}_+, A_0) \implies f \in \mathcal{H}_{t+1}(\mathbb{R}_+, A_0) \quad (6.20)$$

for $0 \leq t \leq n$. Next consider $f \in L^2(\mathbb{R}_+, H)$ with

$$D_0^*f = g \in \mathcal{H}_s(\mathbb{R}_+, A_0), \quad Pf(0) = 0.$$

From part (1) we infer $f \in \mathcal{H}_{s+1,\text{loc}}((0, \infty), A_0)$ and from

$$\begin{aligned} D_{P,\psi}^*\varphi f &= \gamma\varphi'f + \varphi D_{P,\psi}^*f \\ &= \gamma\varphi'f + \varphi D_0^*f \in \mathcal{H}_s(\mathbb{R}_+, A_0), \end{aligned} \quad (6.21)$$

we infer, in view of (6.20), that $\varphi f \in \mathcal{H}_{\min(n,s)+1}(\mathbb{R}_+, A_0)$ and hence $f \in \mathcal{H}_{\min(n,s)+1}(\mathbb{R}_+, A_0)$.

Since n is arbitrary we have proved that the operator $D_{0,P}$ satisfies (4.14) and hence from Theorem 4.13 we conclude that the pair (P, P_+) is elliptic.

Specializing this proof to $s = 0$ immediately implies (2ii). The theorem is proved. \square

REMARK 6.6. An alternative proof of the first part of this theorem could have been given by means of an operator valued pseudodifferential calculus as in [13, Sec. 2].

The regularity at 0 or 1 of \tilde{D} resp. D_P can be obtained under weaker assumptions. We record the results and leave the details to the reader.

THEOREM 6.7. *If we replace (6.2a,b) by*

$A(x) \in \text{Op}^1(A_0)$ and $x \mapsto A(x)(I + A_0^2)^{-1/2}$ is continuous,

then the following hold.

- (1) *\tilde{D} is essentially self-adjoint and $\mathcal{D}(\overline{\tilde{D}}) = \mathcal{H}_1(\mathbb{R}, A_0)$; in particular, \tilde{D} is regular at 0.*
- (2) *Let $P \in \text{Op}^0(A_0)$ be a regular γ -symmetric orthogonal projection. Then D is self-adjoint on*

$$\mathcal{D}(D_P) := \mathcal{D}(D_{0,P}) = \{f \in \mathcal{H}_1(\mathbb{R}_+, A_0) \mid Pf(0) = 0\}.$$

THEOREM 6.8. *If we replace (6.2a,b) by*

$A(x), A'(x) \in \text{Op}^1(A_0)$ and $x \mapsto A(x)(I + A_0^2)^{-1/2}$ is in $C^1(\mathbb{R}, \mathcal{L}(H_0))$,

then the following hold.

- (1) *\tilde{D}^2 is essentially self-adjoint and $\mathcal{D}(\overline{\tilde{D}^2}) = \mathcal{H}_2(\mathbb{R}, A_0)$. In particular, \tilde{D} is regular at 0 and 1.*
 - (2) *Let $P \in \text{Op}^0(A_0)$ be a 2-regular γ -symmetric orthogonal projection. Then*
- $$\mathcal{D}(D_P^2) = \mathcal{D}(D_{0,P}^2) = \{f \in \mathcal{H}_2(\mathbb{R}_+, A_0) \mid Pf(0) = 0, P(Df)(0) = 0\}.$$

7. Well-posed boundary value problems

In this section we consider the situation described in Sec.1.B. We assume that A is a symmetric elliptic differential operator of first order acting on $C^\infty(E_N)$, and that γ is a bundle endomorphism such that (1.9) holds. Then D in (1.10) is an elliptic differential operator on the cylinder $M = \mathbb{R}_+ \times N$. Also, the axioms (3.31) are satisfied with $\Psi^0(A) = \Psi_{\text{cl}}^0(E \upharpoonright N)$. For $\xi \in T_x^*(N)$ denote by $N_\pm(\xi)$ the space spanned by eigenvectors of $\hat{A}(\xi)$ with positive and negative eigenvalues, respectively, where $\hat{A}(\xi)$ denotes the leading symbol.

According to Seeley [28, Def. VI.3], a classical pseudodifferential operator P of order 0 on $C^\infty(E_N)$ is called *well-posed* if

- (i) $P : H_s(E_N) \rightarrow H_s(E_N)$ has closed range for each $s \in \mathbb{R}$;
- (ii) for each $\xi \in T_x^*N \setminus \{0\}$ the principal symbol $\hat{P}(\xi)$ maps $N_+(\xi)$ injectively onto the range of $\hat{P}(\xi)$.

P can always be replaced by an orthogonal projection with the same null space [28, Lemma VI.3], hence defining the same boundary condition. Our aim is to give a functional analytic characterization of well-posedness for orthogonal projections.

PROPOSITION 7.1. *Let P and Q be orthogonal projections in $L^2(E_N)$ which are classical pseudodifferential operators of order 0 on $C^\infty(E_N)$, and denote by \hat{P}, \hat{Q} their principal symbols. Then (P, Q) is a Fredholm pair if and only if for each $\xi \in T_x^*M \setminus \{0\}$*

$$\hat{Q}(\xi) : \text{Im } \hat{P}(\xi) \longrightarrow \text{Im } \hat{Q}(\xi) \quad (7.1)$$

is an isomorphism.

PROOF. Assume that (P, Q) is Fredholm. Then, by Prop. 3.3, $P - Q \pm 1$ is Fredholm and hence also elliptic (cf. eg. [21, Ch. 19.5]). Thus for $\xi \in T^*N \setminus \{0\}$ the endomorphisms

$$\hat{P}(\xi) - \hat{Q}(\xi) \pm 1 \quad (7.2)$$

are invertible. Now we apply Corollary 3.4 to see that the map (7.1) is invertible.

Conversely, if (7.1) is invertible then $(\hat{P}(\xi), \hat{Q}(\xi))$ is a finite-dimensional Fredholm pair and the maps in (7.2) are invertible in view of (3.3), hence $P - Q \pm 1$ is elliptic. Invoking again Prop. 3.2, we conclude that (P, Q) is Fredholm. \square

Condition (i) above is automatic for a pseudodifferential idempotent. Hence, applying this proposition to the pair (P, P_+) immediately gives

THEOREM 7.2. *Let P be a classical pseudodifferential operator of order 0 which is an orthogonal projection. Then P is well-posed if and only if (P, P_+) is a Fredholm pair.*

Finally, we give the

PROOF OF THEOREM 1.5. We use the notation of Section 1.D. By (1.27)–(1.29) and Lemma 1.1 we have

$$\Phi D\Phi^* = \gamma \left(\frac{d}{dx} + A(x) \right) + V(x).$$

We choose a function $\psi \in C_0^\infty(-\varepsilon_0, \varepsilon_0)$, $0 \leq \psi \leq 1$, with $\psi = 1$ near 0 such that the operator

$$A_\psi(x) = \psi(x)A(x) + (1 - \psi(x))A_0 \quad (7.3)$$

is elliptic for all $x \geq 0$, which is certainly the case if the support of ψ is small enough. Then we introduce the operator

$$D_\psi := \gamma \left(\frac{d}{dx} + A_\psi(x) \right) \quad (7.4)$$

and note that D_ψ satisfies (6.1) and (6.2). We will prove the following

CLAIM. *The operator D_P is self-adjoint if and only if the operator $D_{P,\psi} := D_\psi^* \upharpoonright \{f \in \mathcal{H}_1(\mathbb{R}_+, A_0) \mid Pf(0) = 0\}$ is self-adjoint.*

Theorem 1.5 is an immediate consequence of the Claim:

Since the algebra $\Psi_{\text{cl}}^0(E_N)$ satisfies the assumptions (1.19) (cf. the discussion before Theorem 1.3) and since the elliptic operator A_0 is discrete we infer from Theorem 5.6 that the Fredholmness of the pair (P, P_+) is equivalent to the ellipticity of the pair (P, P_+) resp. to the regularity of P .

From the Regularity Theorem 6.5 (2ii) we thus know that $D_{P,\psi}$ is self-adjoint if and only if the pair (P, P_+) is Fredholm. In view of Theorem 7.2 this, in turn, is equivalent to the fact that P is well-posed in the sense of Seeley. Again, from the Regularity Theorem 6.5 and Theorem 1.4 we see that the operators Q, K_r, K_l are obtained by patching together an interior parametrix of D and the analogue of (1.25) for $D_{P,\psi}$.

It remains to prove the claim:

First, we note that the operator $V(x)$ is bounded and hence adding or subtracting $V(x)$ does not affect the domain of an operator.

Choose a cut-off function $\chi \in C_0^\infty(-\varepsilon_0, \varepsilon_0)$ such that $\psi = 1$ in a neighborhood of $\text{supp } \chi$. Assume first that D_P is self-adjoint and let $f \in \mathcal{D}(D_{P,\psi}^*)$. By the same calculation as in (6.21) one shows $\chi f \in \mathcal{D}(D_{P,\psi}^*)$, hence by construction we have $\Phi^*(\chi f) \in \mathcal{D}(D_P^*) = \mathcal{D}(D_P)$. Thus, by (1.29), we have $\chi f \in \mathcal{D}(D_{P,\psi})$. The proof of the converse is similar. The Claim and hence the Theorem are proved. \square

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